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DOPPLER-LIMITED SPECTRUM OF HIGH TEMPERATURE WATER VAPOR IN THE--ETC(U)
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MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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DOPPLER-LIMITED SPECTRUM OF HIGH TEMPERATURE WATER VAPOR IN THE 3000 TO 4000 cm^{-1} REGION

10 Allan S. PINE

Group 82

FINAL REPORT

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Abstract

The absorption spectrum of water vapor has been recorded at very high temperatures ($\sim$ 1200 K) in the 3000 to 4000 cm^{-1} region with Doppler-limited resolution using a tunable difference-frequency laser spectrometer. This region encompasses the strong OH stretching fundamentals and the bending overtone. The higher rotational and vibrational energy levels observed here are expected to lead to extended theoretical models of H_2O which are necessary to predict and analyze spectra from high temperature combustion processes.

Contents

Introduction

The high temperature absorption spectrum of water vapor has been recorded in the 3000 to 4000 cm^{-1} region with Doppler-limited resolution using a tunable difference-frequency laser spectrometer. This spectral region contains the strong ν_1 and ν_3 OH stretching fundamentals and the $2\nu_2$ bending overtone. At the temperatures of this experiment (~ 1200 K) the ν_2 vibration is highly excited so that many hot band lines as well as higher rotational levels are observed. The purpose of this study is to extend the hot band and high J rotational assignments for H_2O and to obtain precision transition wavenumbers and intensities for refining the theoretical models. Water vapor, of course, is an oxidation product of the burning of hydrocarbons and other fuels and an accurate knowledge of its high temperature spectrum is an aid in combustion diagnostics.

The water vapor spectrum at low temperatures (~ 300 K) is quite well known with the high-resolution Fourier transform interferometer study by Camy-Peyret, Flaud, Guelachvili and Amiot [1] being perhaps the most complete and precise to date. This FTS study [1] is our primary reference for calibration and comparison. At high temperatures the most extensive study is the H_2O emission spectrum from an H_2/O_2 flame by Flaud, Camy-Peyret and Maillard [2], also recorded on a Fourier transform instrument. Temperatures in the flame reached 2900 K which are much higher than can be obtained in absorption cell experiments. However, the complex temperature distribution in the flame and its atmospheric pressure operation create some uncertainties in measurements of line intensities and positions. Thus it seems appropriate to perform a controlled, low pressure absorption experiment at intermediate temperatures to bridge the gap between the cold water and flame measurements in order to confirm and extend assignments and to improve the data precision on which the theoretical models are based.

Experimental Details:
Instrumental Considerations

The tunable laser Difference-Frequency Spectrometer used to record the Doppler-limited spectrum of high temperature water vapor is shown schematically in Fig. 1. Here a cw single-mode argon and tunable dye laser are mixed in the nonlinear optical crystal $LiNbO_3$. The infrared beat frequency generated in the $LiNbO_3$ crystal is split into sample and reference beams for ratio recording to eliminate amplitude fluctuations due to the incident lasers. The AR-coated Ge filters in front of the InSb detectors pass the IR and eliminate the visible whereas the liquid water cell before the $LiNbO_3$ filters out the incoherent IR generated by the ion laser discharge. Critical phasematching at 90° to the $LiNbO_3$ optical axis is achieved by temperature tuning the oven-controlled crystal. Details on the visible-to-infrared conversion efficiency, spectral coverage, phasematching requirements, drift compensation, extended scan range, stabilization and linear scan control of the Difference-Frequency Spectrometer appear in references [3,4,5,6].

In the present experiment the Difference-Frequency Spectrometer was tuned over the range from 4005 cm^{-1} to 2965 cm^{-1} to encompass the entire fundamental ν_1 and ν_3 bands and the overtone $2\nu_2$ of water vapor. This coverage of more than 1000 cm^{-1} at ultrahigh resolution (instrumental linewidth $\sim 3 \times 10^{-4}$ cm^{-1}, Doppler linewidth $\sim 2 \times 10^{-2}$ cm^{-1}) is by far the most extensive continuous scan yet achieved with a tunable infrared laser. The spectrum was recorded in 3.75 cm^{-1} segments overlapped at 3.0 cm^{-1} intervals. Each segment required 5 minutes to scan using a time constant of 40 msec chosen to provide good signal-to-noise (~ 300:1) and a full response to sharp spectral features. The data were digitized at a 20 Hz rate (~ 6×10^{-4} cm^{-1} grid) and stored on magnetic tape for subsequent computer processing. A microprocessor-based tape data logger was specially constructed for this experiment for dedicated, reliable, high-density mass storage with a local memory buffer and manual baseline digitizer feature. Our previous data acquisition scheme involved direct transmission of the digitized spectrum to the main laboratory computer via an interactive device coupler. However, that access was too limited and intermittent for

this experiment which required extremely long runs at very high sample temperatures. A photograph of the data acquisition system is shown in Fig. 2.

The manual baseline digitizer feature was incorporated to correct for pathological baseline variations due to strong atmospheric water vapor absorptions which occur within the H_2O range scanned. It was not possible to evacuate the infrared section of the Difference-Frequency Spectrometer; however open atmospheric paths were reduced by inserting cells filled with dry N_2 gas. Some H_2O lines are so strong though, that even a few centimeters of atmospheric path absorbs most of the light in the sample and reference beams, creating a very noisy spectrum. In addition, the experiment was conducted in the winter months for lowest humidity since the laboratory air-conditioning does not significantly reduce the humidity in the summer.

The residual baseline variations in principle could be treated in various ways. Ideally, one would record both a full cell and an empty cell trace for normalization. However, the hot water cell could not be readily evacuated since it was sealed-off and the vapor pressure was regulated through a temperature-controlled side-arm ice reservoir. Also this normalization method would have doubled the data recording time and storage requirements which would be prohibitive due to the extensive spectral coverage. A second normalization method would be to balance the open atmospheric paths in the sample and reference beams so that the ratio recording would eliminate the atmospheric background variation. Unfortunately the double-passed high temperature sample cell geometry required a minimum open path of $\sim$ 20 cm, and this long a path in the reference beam would have caused the ratio-denominator to approach zero for too many lines. Thirdly numerical methods could have been used to estimate the baseline by distinguishing between sharp Doppler-limited low pressure transitions and slow background variations due to broad atmospheric absorptions. This is our usual approach for generating baselines for molecular spectra outside the H_2O region. However, the algorithm does not work satisfactorily for the strong, relatively sharp, baseline variations due to atmospheric water vapor absorptions which were of course in close coincidence with many of the lines under investigation. For all these practical reasons we chose to determine the

baselines interactively with a manual baseline digitizer incorporated in the data logger electronics using a storage CRT display. An example of the sampled baseline on a transmission trace is shown in Fig. 3.

The observed signal-to-noise ratio of ~ 300:1 was limited in this experiment by background noise generated by the high temperature sample cell. For ordinary room temperature cells the instrumental signal-to-noise ratio is ~ 1000:1. The hot cell creates two excess noise sources - thermal background radiation and atmospheric convection currents. Since the oven and cell walls at 1200 K are glowing red hot it is necessary to prevent this radiation from reaching the sample detector. This was accomplished by extending the hot cell windows outside the oven and optically masking the walls by focusing and spatially filtering the infrared laser beam. This was found to be more effective than spectral filtering using a broad band tunable interference wedge which caused additional attenuation. Convection currents in the heated air outside the hot cell windows created excess noise by shifting the infrared beam around on the active detector surface. This problem was reduced by inserting draft-shielding tubes against the cell windows. Evacuable antechambers would have been preferable but were prevented by the oven configuration.

Transition wavenumbers were obtained by linear interpolation between fringes of a high finesse scan calibration interferometer monitoring the visible lasers as shown in Fig. 1. This interferometer was referenced to a Lamb-dip stabilized He/Ne laser which maintained the calibration and resettability to ~ 5 x 10^{-4} cm^{-1} during the entire course of the experiment (~ 1 month). The calibration of the index frequency, free-spectral-range and dispersion of the interferometer was accomplished by reference to the room temperature H_2O Fourier-transform study by Camy-Peyret <u>et al</u>. [1]. Here cold water spectral excerpts were recorded about every 100 cm^{-1}. Clean, isolated reference lines were selected and the Fabry-Perot fringes were least-squares fit to a parabola. The correct interorder number could be estimated from previous precision measurements [3] of the free-spectral-range and were verified by the continuous scan of the high temperature H_2O spectrum. The fit resulted in a calibration curve of

$$\omega_N = \omega_0 - N x (FSR - N x DISP)$$

where N is the interorder number, ω_0 = 4005.19963 cm^{-1}, FSR = 0.0500316 cm^{-1} and DISP = 1.6136×10^{-10} cm^{-1}. The dispersion (variation of the free-spectral-range) is quite noticeable over the extensive tuning range covered in this experiment ($N_{MAX} \sim 21000$). It results principally from wavelength-dependent phase shifts in the double-stack broad-band multidielectric reflective coatings of the scan calibration interferometer and to a lesser extent from the dispersion of air over the dye laser tuning range.

Sample and Cell Considerations

The absorption cell used in this experiment was a 4.1 cm diameter fused quartz tube with 3 mm thick GE125 fused quartz Brewster angle windows glass blown on to the ends of the tube. These windows are relatively water-free, exhibiting only ~ 3% broad-band absorption between 3600 and 3700 cm^{-1}. A ~ 10 cm long quartz side arm was blown onto the tube near one end for pump-out, fill and seal-off and for containing the sample reservoir during the experiment. The cell was approximately 130 cm long with the ends protruding equally from either side of the 90 cm long tube furnace.

The Marshall furnace consisted of a 30 cm and a 60 cm section mounted end-to-end with a 5.1 cm bore and a 6.5 cm insulating wall. The furnace was rated at 1100°C and was operated at ~ 927°C during this experiment. Temperature was measured with two platinum/platinum-13% rhodium thermocouples and a digital readout (Doric 412A Trendicator, nominal calibration accuracy ± 0.6°C). Temperature was maintained manually ± 1°C using Variac controls on the AC power to the ovens after about a 3 hr. warm-up each day. A schematic of the oven and cell and the measured temperature profile is shown in Fig. 4. There is a slight drop in temperature at the junction of the two ovens and much larger gradients near the ends of the oven. The cell extends through the gradient region out to room temperature in order to avoid the excess noise problems associated with hot windows as discussed previously.

The water vapor pressure is maintained constant throughout the cell by controlling the temperature of the H_2O ice reservoir in the side arm. The cold bath contained a ~ 40% ethylene glycol in water antifreeze solution adequate for cooling to below -20°C by passing cold liquid nitrogen boil-off gas through an immersed copper coil. The antifreeze was temperature regulated with an immersed resistance heater to ± 0.2°C. For the spectral region above ~ 3270 cm^{-1} where the water vapor absorptions are strongest, the bath temperature was -20 ± 0.2°C corresponding to a vapor pressure of 0.776 ± 0.015 Torr. Below 3270 cm^{-1} a reservoir temperature of -10 ± 0.2°C, corresponding to a vapor pressure of 1.95 ± 0.04 Torr, was used to enhance the weaker transitions. In both ranges the cell was double-passed to increase the absorptions.

The water sample itself was freshly distilled and deionized (ρ > 18 MΩ-cm) before filling the cell. Nevertheless both CO_2 and CH_4 impurity lines are observed in the spectrum. These impurity lines were easily recognized by their distinctive patterns and they were sparse enough that there was little interference with the water spectrum. It is believed that the CO_2 was present in the initial water sample due to absorption from the air since the amount of CO_2 increases with the amount of time between distillation and cell filling. The CH_4 only appears after cycling to high temperatures and may involve degassing from the cell walls. A bake-out of the cell under vacuum, however, did not eliminate the methane.

It should also be noted that we initially tried some metal cells constructed of inert, high temperature alloys, Monel 400 and Inconel 600. Metal cells would be more covenient for attaching flanges and demountable IR windows. However, the water vapor reacted with the hot metal walls at temperatures above ~ 550°C and consequently the spectrum disappeared. Plating the cells with rhodium and platinum did not prevent this oxidation. For the much higher temperatures desired for this experiment, the metal cells were abandoned in favor of quartz.

Results and Discussion

The complete high temperature water vapor spectrum recorded between 4005 and 2965 cm^{-1} is presented in Appendix I in overlapping 12.75 cm^{-1} panels. The spectral intensity scale shown is normalized according to Beer's law

$$I(\omega) = (PxL)^{-1} \ln(B(\omega)/S(\omega))$$

where P is the vapor pressure in Torr, L(= 252 cm) is the double-passed cell length, $B(\omega)$ is the baseline corresponding to the empty cell transmission and $S(\omega)$ is the water vapor transmission spectrum. Even though the pressure is uniform throughout the cell, these intensities must be corrected for the variation of density, Doppler width and lower state populations due to the temperature gradients in the cell. For example high temperature lines not seen at room temperature (i.e., hot band and high J transitions) have a shorter effective cell length (~ 136 cm) and twice the Doppler width as a 300 K line. Such linewidth variation is readily observed throughout the spectrum and helps to distinguish the hot lines. Lines seen at both high and low temperatures have a complex lineshape corresponding to the sum of Gaussians weighted by the temperature distribution. Therefore one must proceed with care in analyzing these intensity data for transition moments. This problem is similar to that encountered in atmospheric and plume modeling which are also plagued by complex pressure, density and temperature distributions. In the present case these distributions have at least been measured from the vapor pressure at the cold bath temperature and the cell temperature profile shown in Fig. 4. A theoretical Hamiltonian model, however, is required to determine the Boltzmann populations of the lower levels and the rotational wavefunctions before we can compare the transition moments to the data.

Impurity lines in the spectrum of Appendix I are labelled by an asterisk. Those arising from the $\nu_1+\nu_3$ and $2\nu_2+\nu_3$ combination bands of CO_2 and their associated hot bands are confined to the 3753 to 3554 cm^{-1} region. They are easily distinguished from water vapor lines by their

narrower Doppler width as befitting a heavier molecule. Lines due to the ν_3 band of CH_4 fall below 3200 cm^{-1}. The noisy regions of the spectrum occur locally near very strong atmospheric water vapor absorptions and arise because of the low light level incident on the reference detector.

The wavenumber scale in the spectrum is calibrated against the cold water spectrum of Camy-Peyret et al. [1] as mentioned previously. A listing of the observed line center wavenumbers in cm^{-1} and the measured peak intensities in $(Torr\ m)^{-1}$ is given in Appendix II. The DIFF column is the wavenumber difference in 10^{-4} cm^{-1} for the present data minus prior literature values. The prior references are coded in the CD column. C stands for the cold water data of Camy-Peyret, Flaud, Guelachvili and Amiot, Mol. Phys. 26, 825 (1973). A and B are the theoretical and hand measured frequencies in Ref. C. S represents the very strong cold water lines [INT > 2.0 $(Torr\text{-}m)^{-1}$; off scale on the plots] which were somewhat saturated in the present transmission spectra, so their frequencies and intensities are not given reliably. H represents the high-temperature flame-spectra water vapor emission lines observed by Flaud, Camy-Peyret and Maillard, Mol. Phys. 32, 499 (1976); the unpublished listing was obtained from J.-M. Flaud. D corresponds to the theoretical line positions of carbon dioxide combination bands by Gordon and McCubbin, J. Mol. Spectrosc. 19, 137 (1966) [7]. M corresponds to methane line frequencies given by Tarrago, Dang-Nhu, Poussigue, Guelachvili and Amiot, J. Mol. Spectrosc. 57, 246 (1975) [8]. Those methane lines not included in Tarrago et al. were identified with reference to Gray, Robiette and Pine, J. Mol. Spectrosc. 77, 440 (1979) [9] but no frequency comparisons were made.

There are many lines that appear in the spectral plots that are not listed because the peak finding routine rejects lines that are too weak, too strong or too broad. The weak lines are eliminated in order to discriminate against noise; the strongest lines are completely saturated and the broad lines are usually blends or shoulders whose frequencies would not be determined accurately by the program. The program may also generate slight errors on asymmetric lines such as those due to incompletely resolved K-doublets with 3:1 statistical weights. Similarly partially resolved blends may create errors since the curve-resolving routine

requires lines of uniform width and Gaussian shape whereas the data include various shapes and widths due to hot and cold lines and impurities.

The instrumental precision of the difference-frequency spectrometer is dominated by the least reading (or digitizing grid) and is $\sim 6 \times 10^{-4}$ cm^{-1}. The performance here may be somewhat degraded because of the water vapor sample itself. Here the Doppler widths are relative large because of the light molecule and high temperatures. The background is noisier than usual due to black body thermal emission from the hot cell walls and to the hot air convection currents moving the infrared beam around outside the cell. Also the atmospheric water vapor absorption creates a pathological baseline that causes noise and distortion near strong lines.

The error distributions for the cold and hot water and methane lines are shown in Figs. 5, 6 and 7. For cold water we have taken all lines labelled C and ignored those labelled A, B and S to obtain an average deviation of -0.47×10^{-4} cm^{-1} and an rms deviation of 8.25×10^{-4} cm^{-1}. For the flame spectra labelled H, we obtain an average deviation of -5.25×10^{-4} cm^{-1} and an rms error of 36.93×10^{-4} cm^{-1}. The methane comparison yields an average shift of -0.82×10^{-4} cm^{-1} and an rms error of 5.47×10^{-4} cm^{-1}, but there are probably not enough methane lines to give good statistics. Of course, these rms deviations are due to random errors in both the present data and the previous measurements. Any systematic errors in the original calibration spectrum C will be reflected in the present measurements. The previous flame spectra of Maillard suffered from even larger linewidths and possible pressure shifts due to operation at atmospheric pressure. Therefore the present hot water data are expected to be considerably more precise ($\sim 1 \times 10^{-3}$ cm^{-1}) than the flame spectra.

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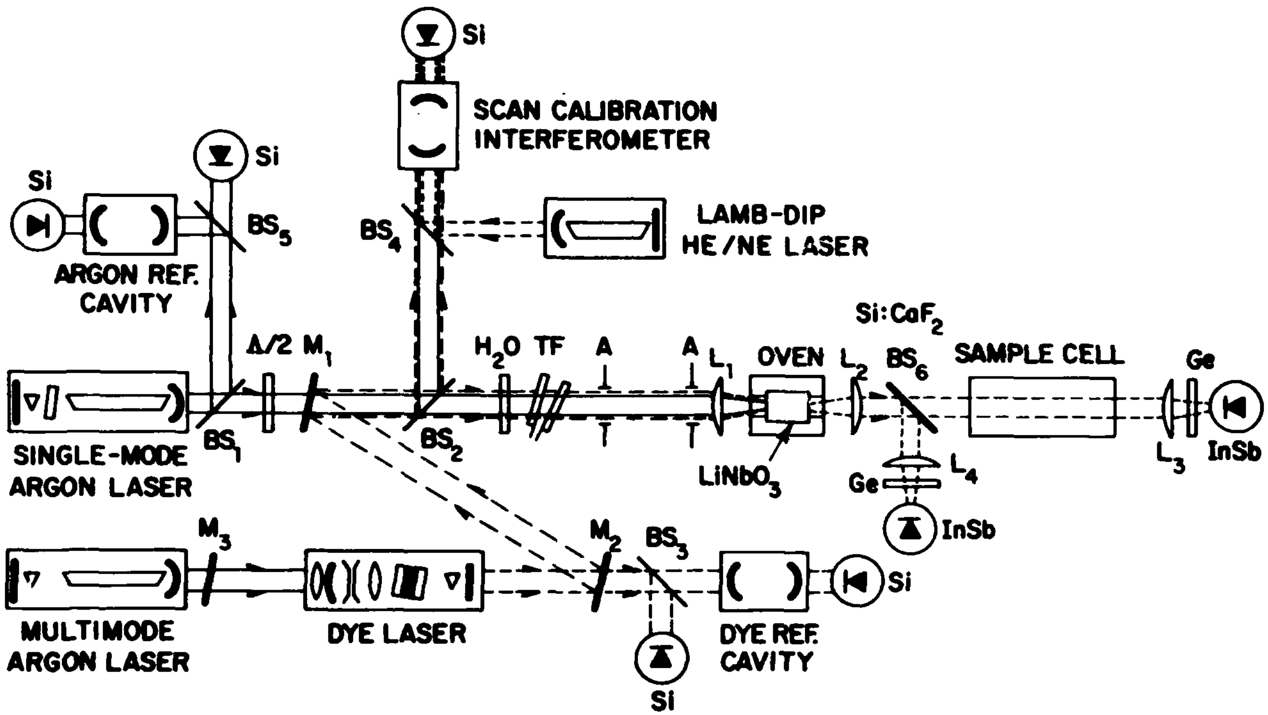


Fig. 1. Optical schematic of the difference-frequency spectrometer. M_i are mirrors, BS_i are beam splitters, L_i are lenses, A are apertures, TF is tuning fork chopper, Si are PIN silicon photodiodes, InSb are photovoltaic IR detectors.

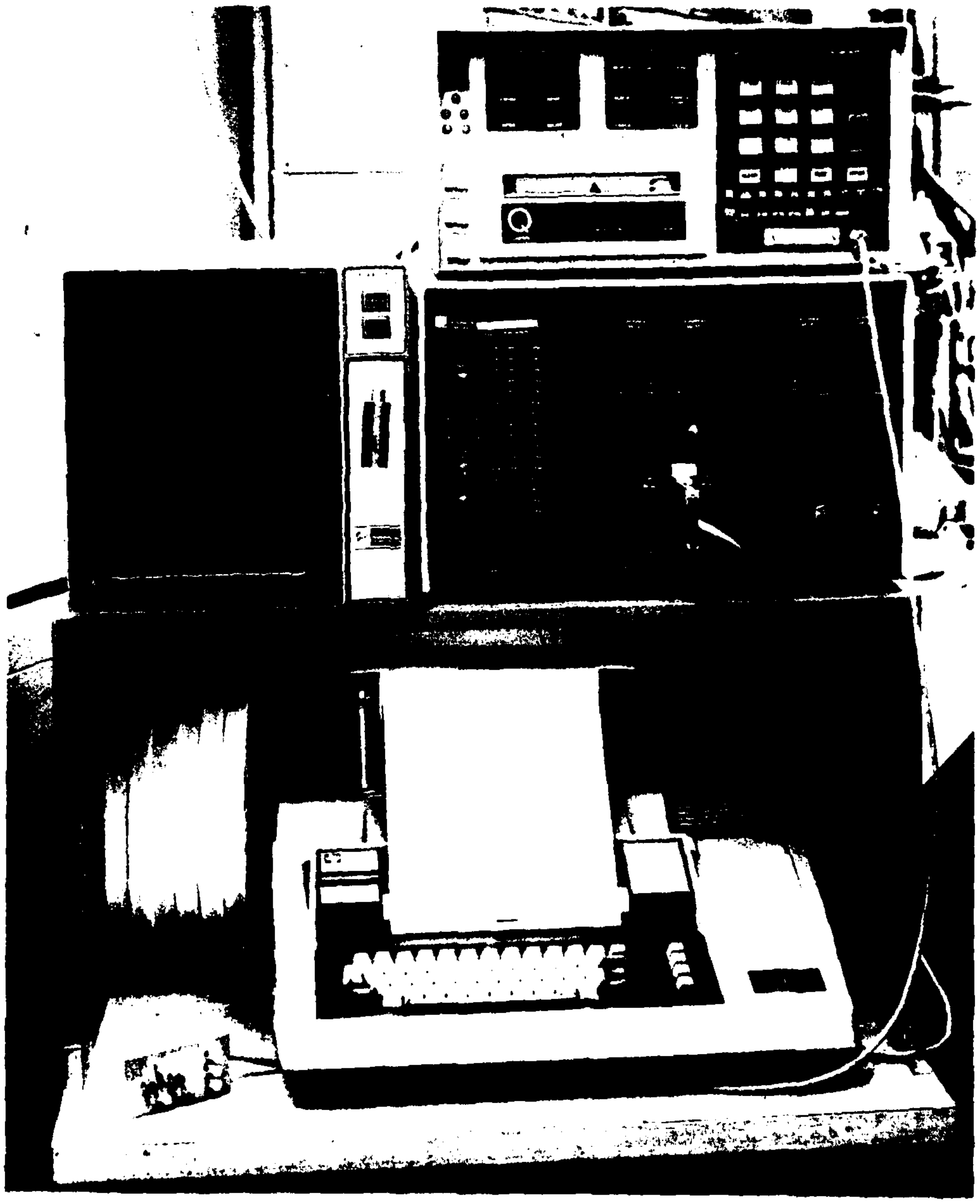


Fig. 2. Data acquisition system. Digitized data stored in memory and tape of tape logger; displayed on storage CRT; interfaced with laboratory computer via device coupler; terminal used to communicate with laboratory computer on time-sharing.

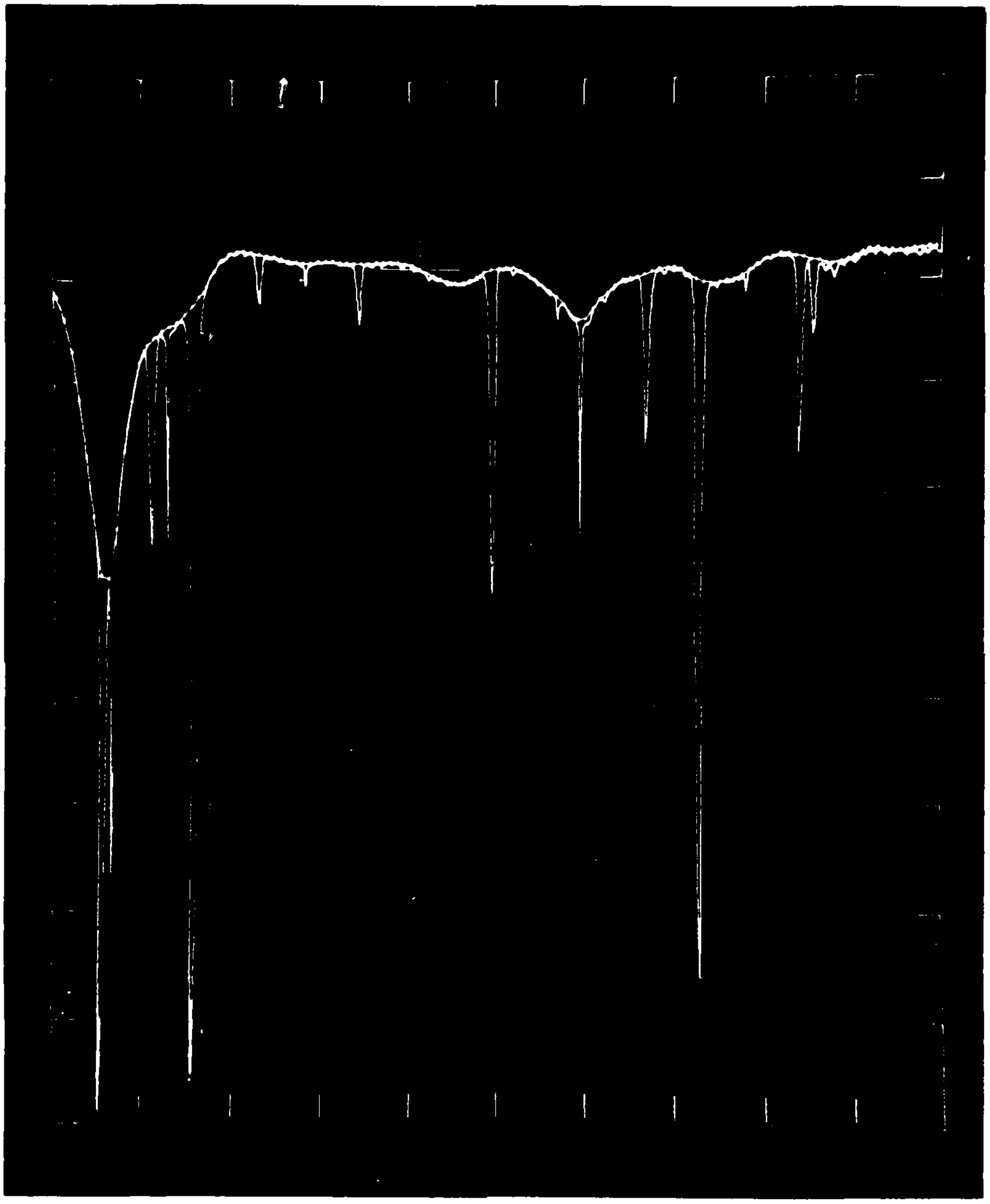


Fig. 3. Interactive baseline digitizer. The dotted curve on the baseline is entered interactively and the baseline is linearly interpolated.

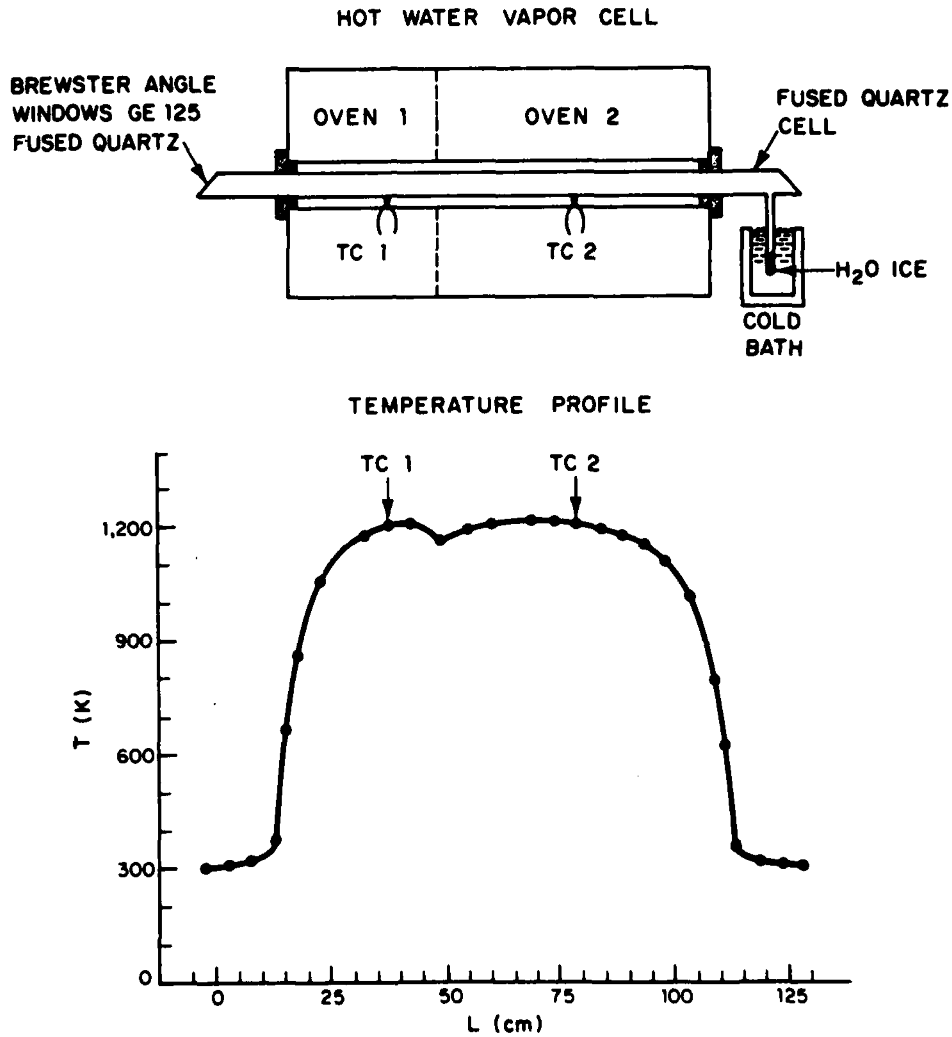


Fig. 4. Sample cell schematic and temperature profile. During scan, thermocouples monitored temperature at peaks of profile at TC1 and TC2, and ovens were controlled individually.

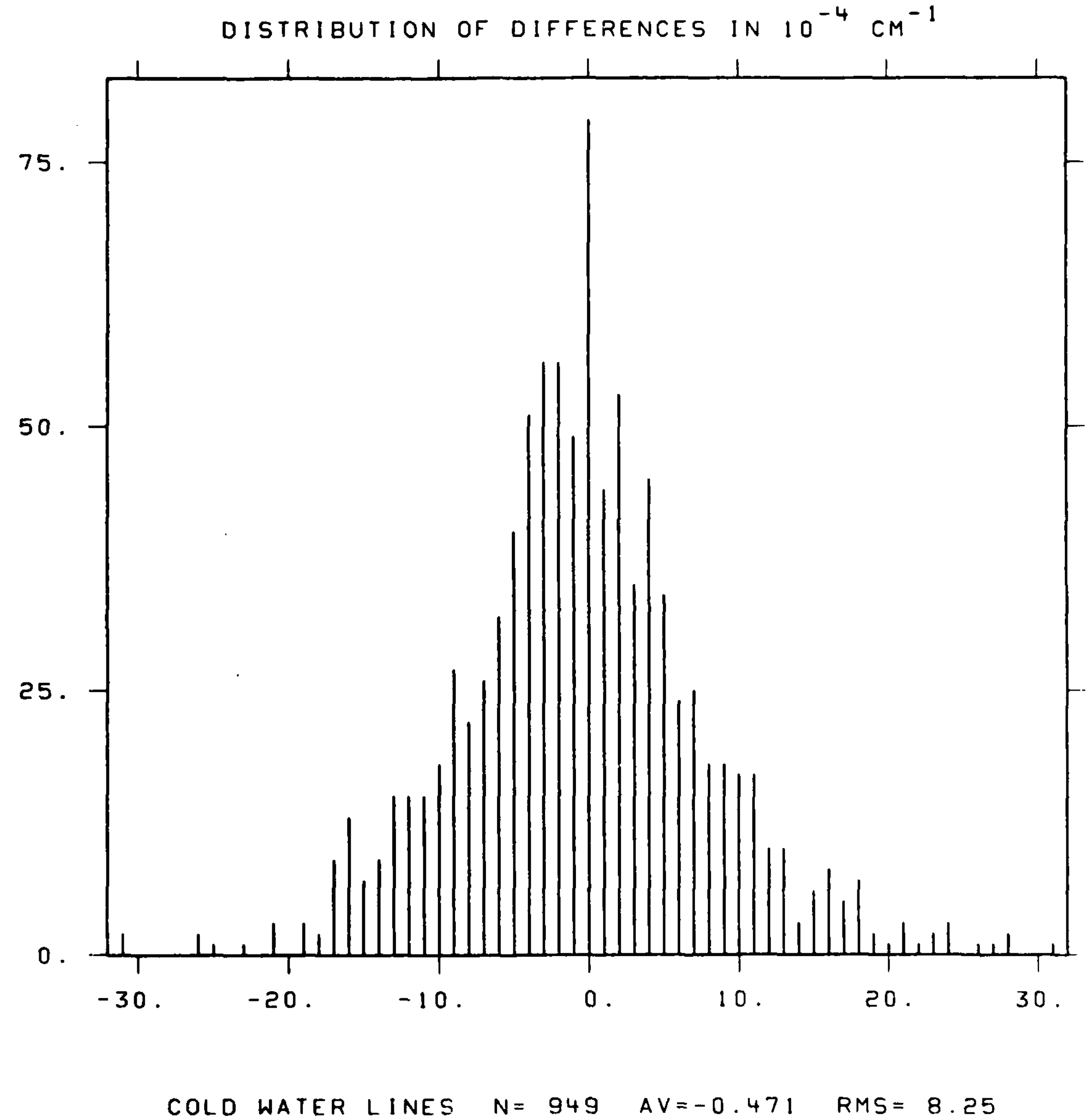


Fig. 5. Comparison differences: present cold water lines minus Ref. C [1]. Differences in units of 10^{-4} cm^{-1}.

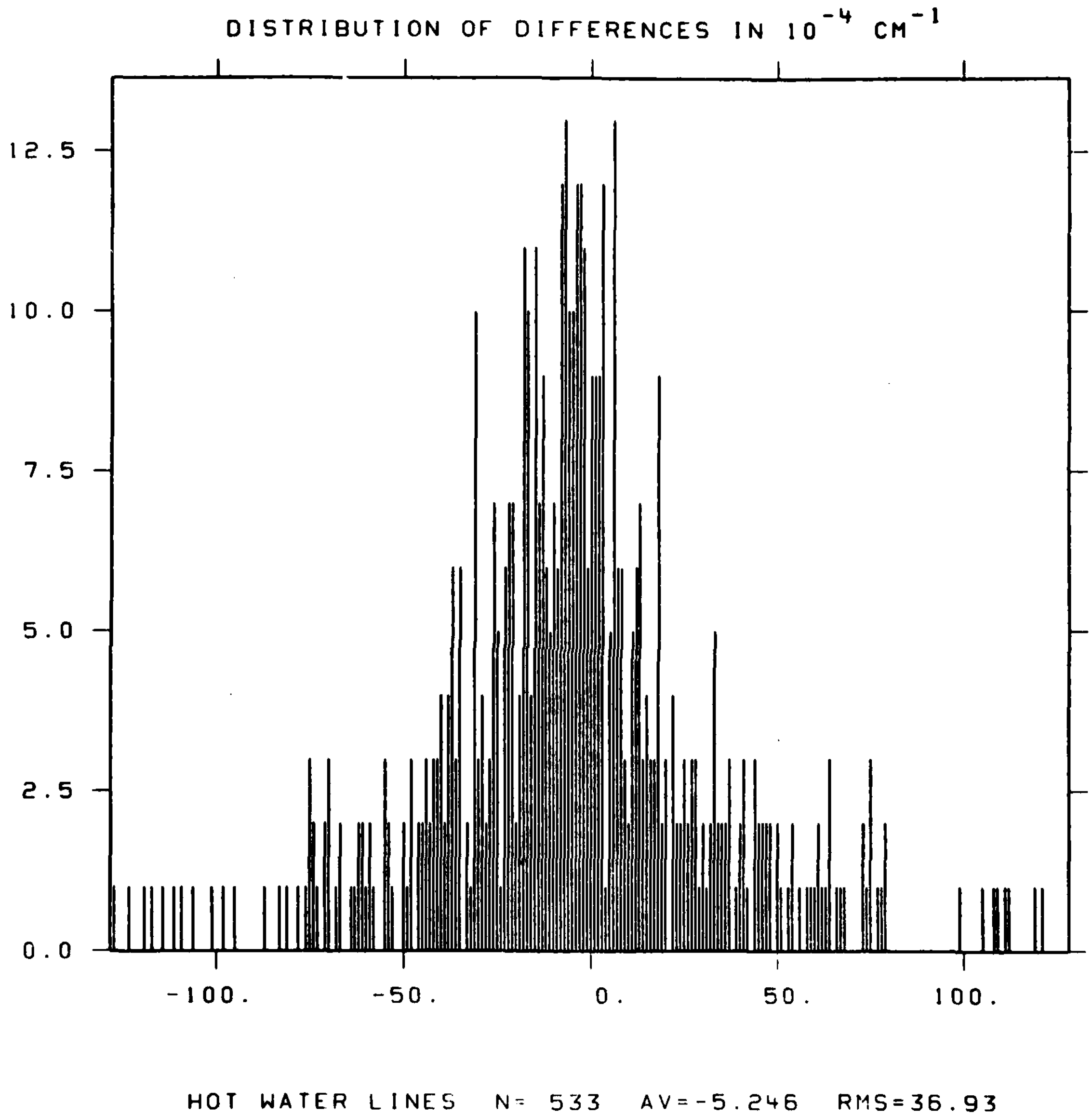


Fig. 6. Comparison differences: present hot water lines minus Ref. H [2]. Differences in units of 10^{-4} cm^{-1}.

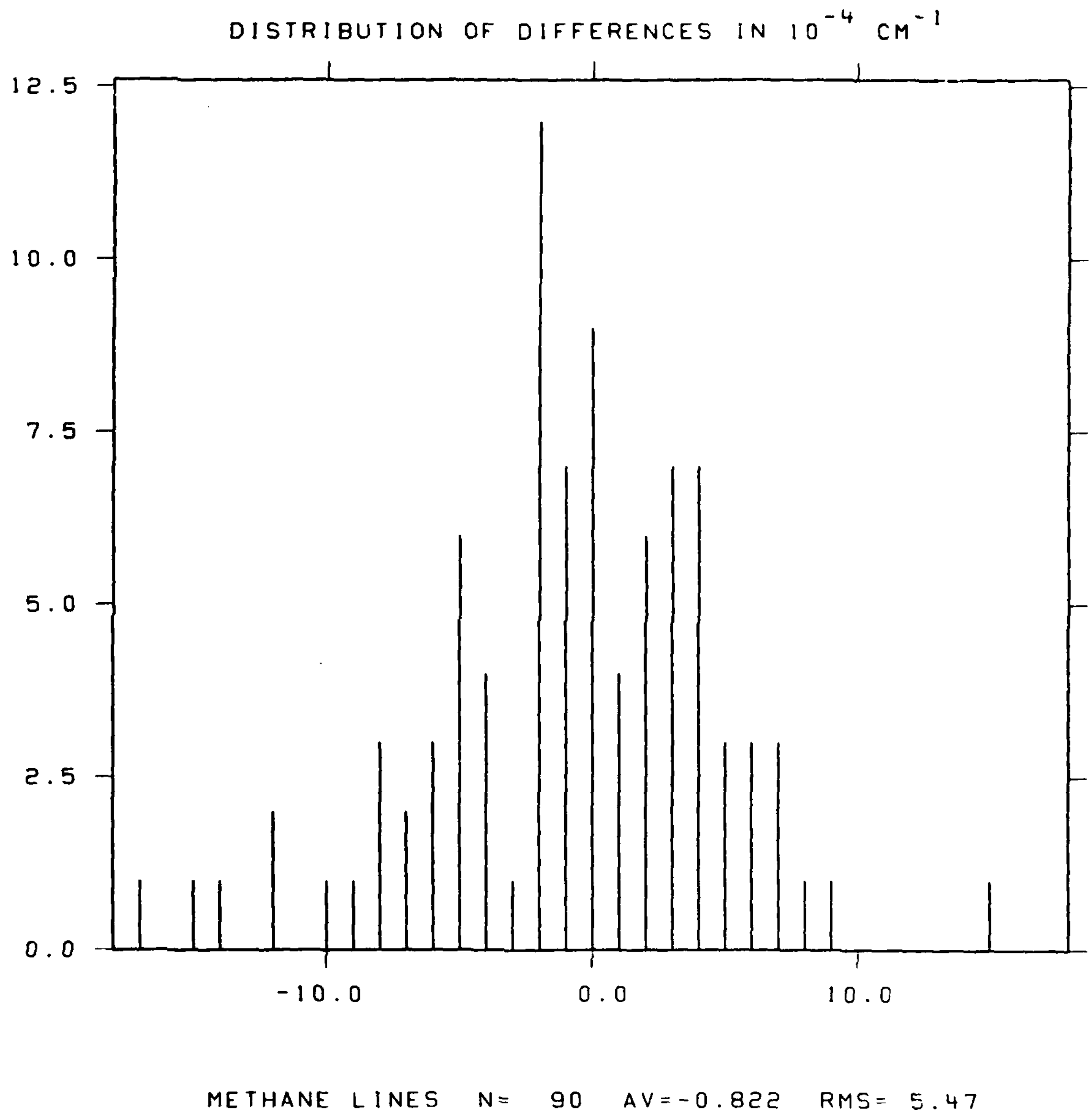
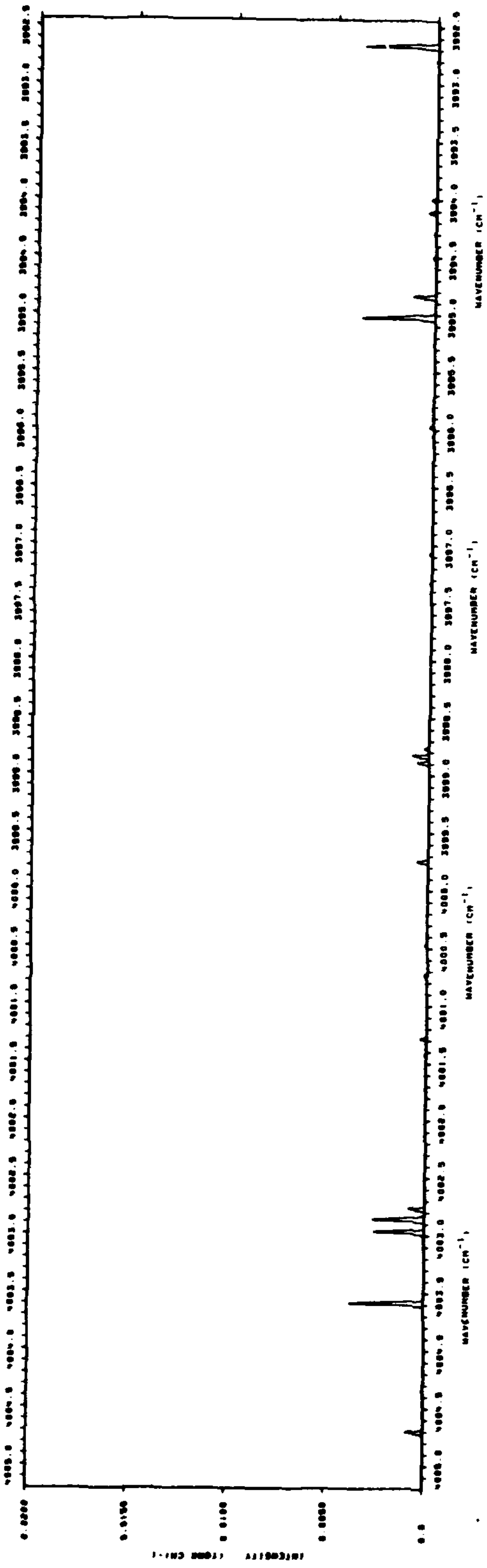
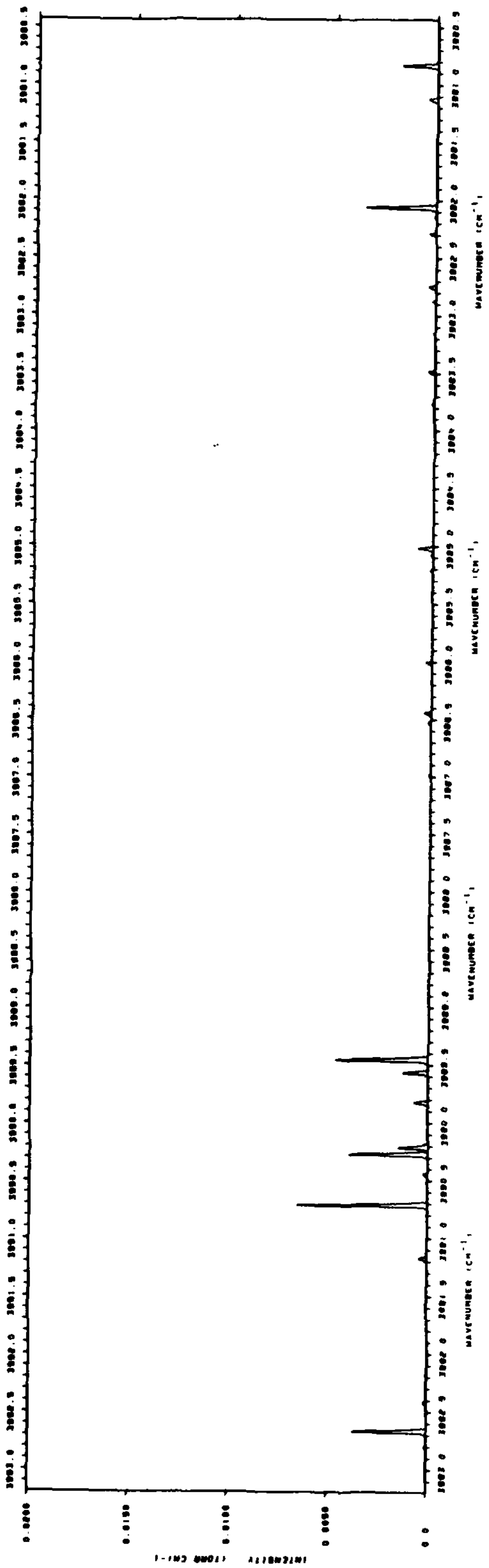


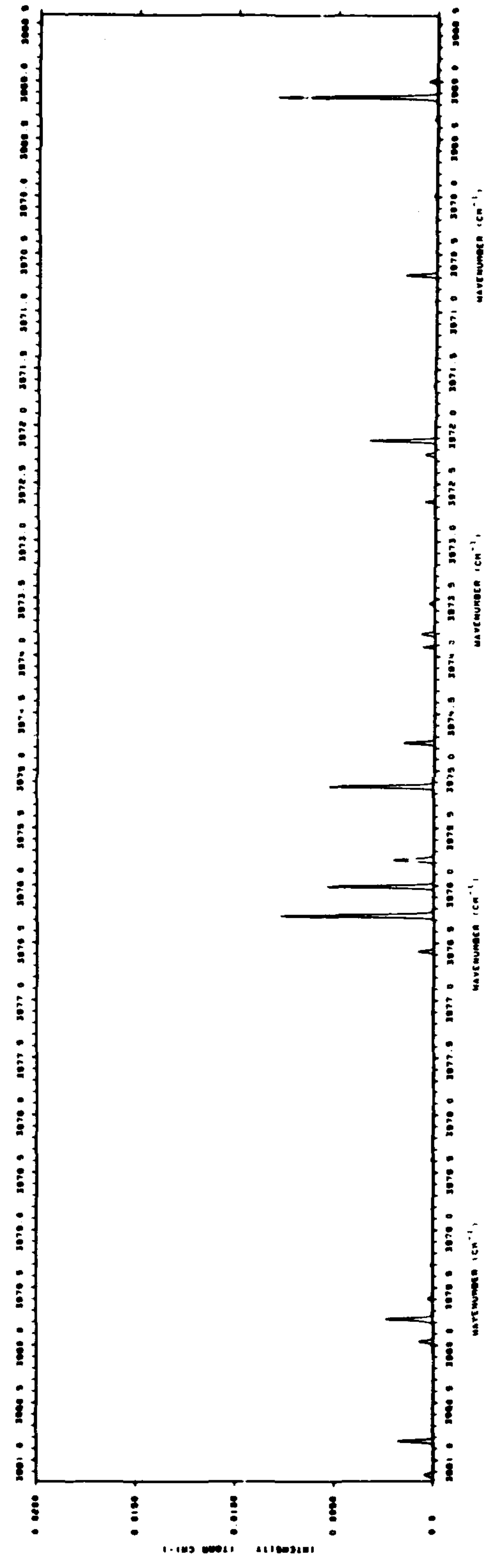
Fig. 7. Comparison differences: present methane lines minus Ref. M [8]. Differences in units of 10^{-4} cm^{-1}.

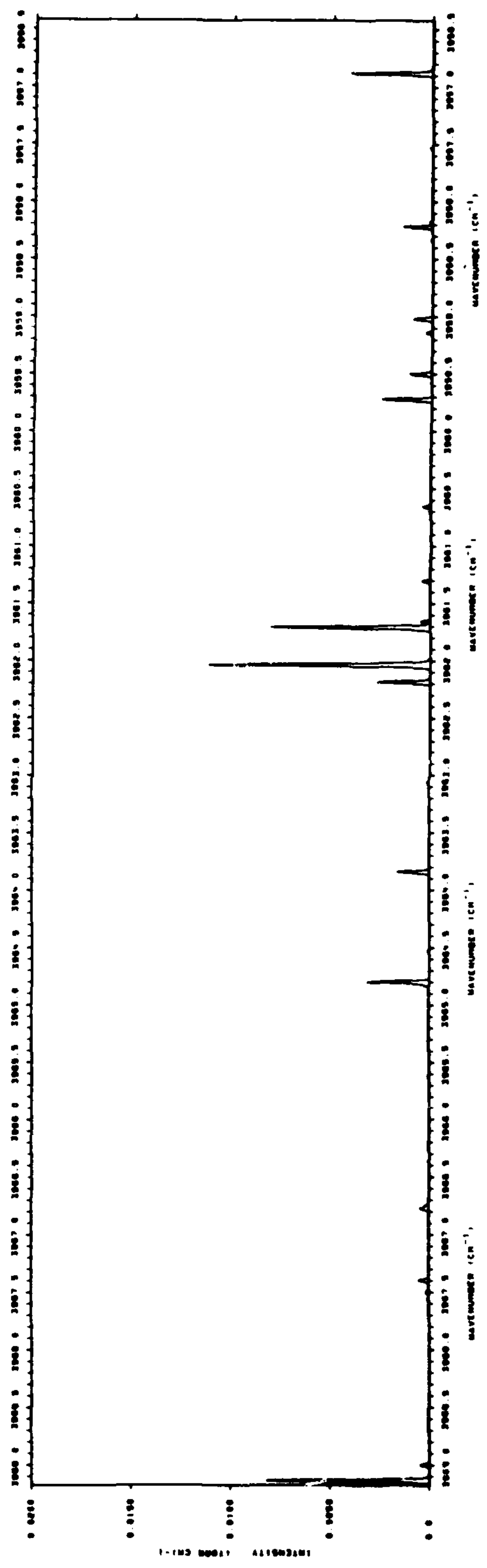
Appendix I.

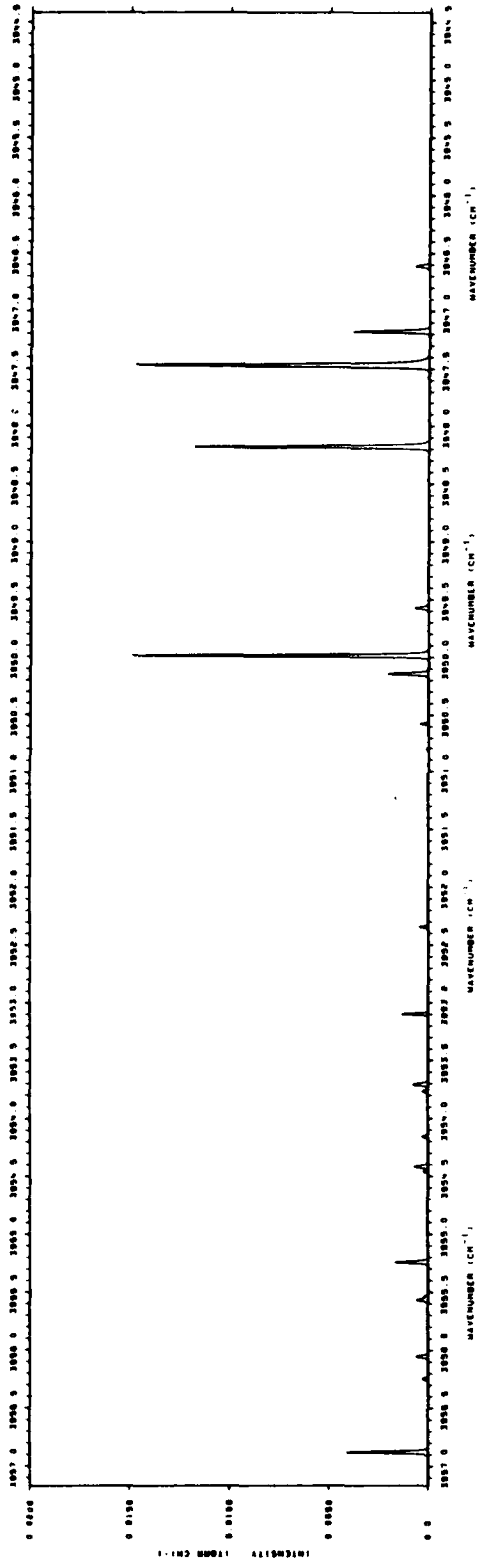
Spectral Plots of High Temperature H_2O

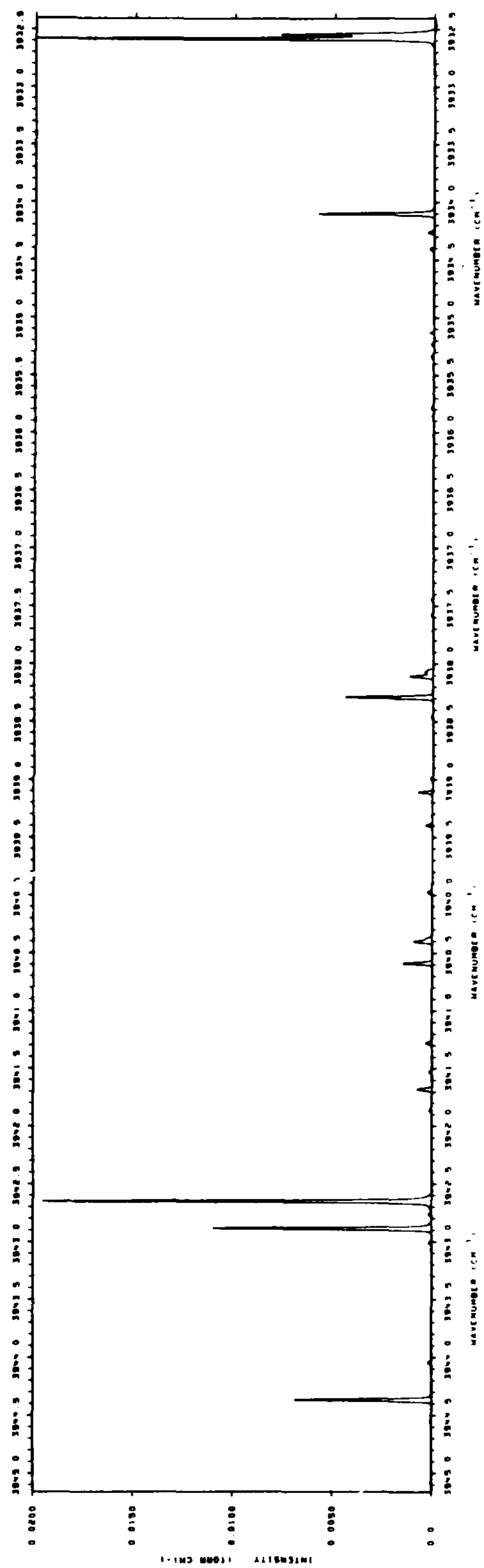


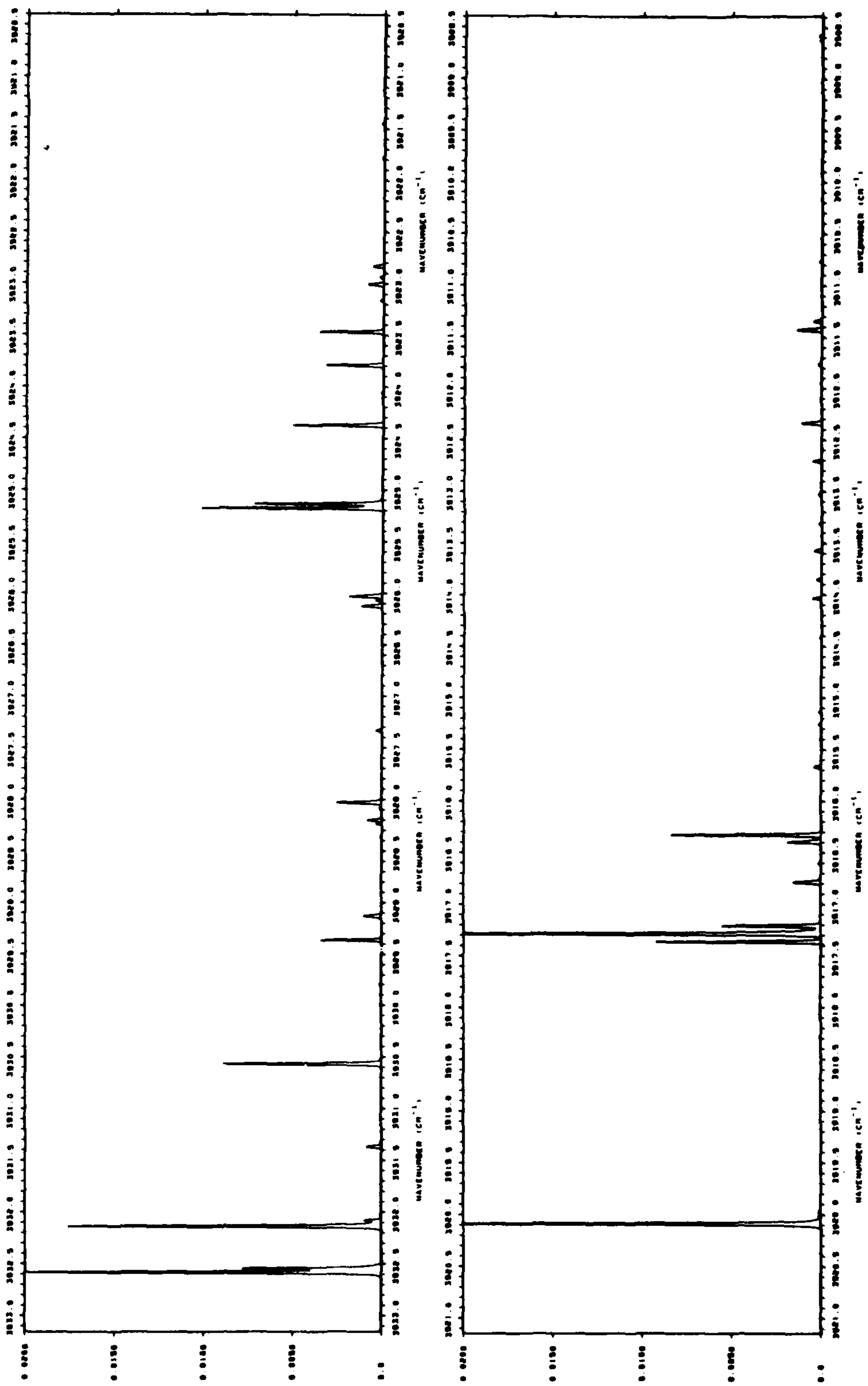


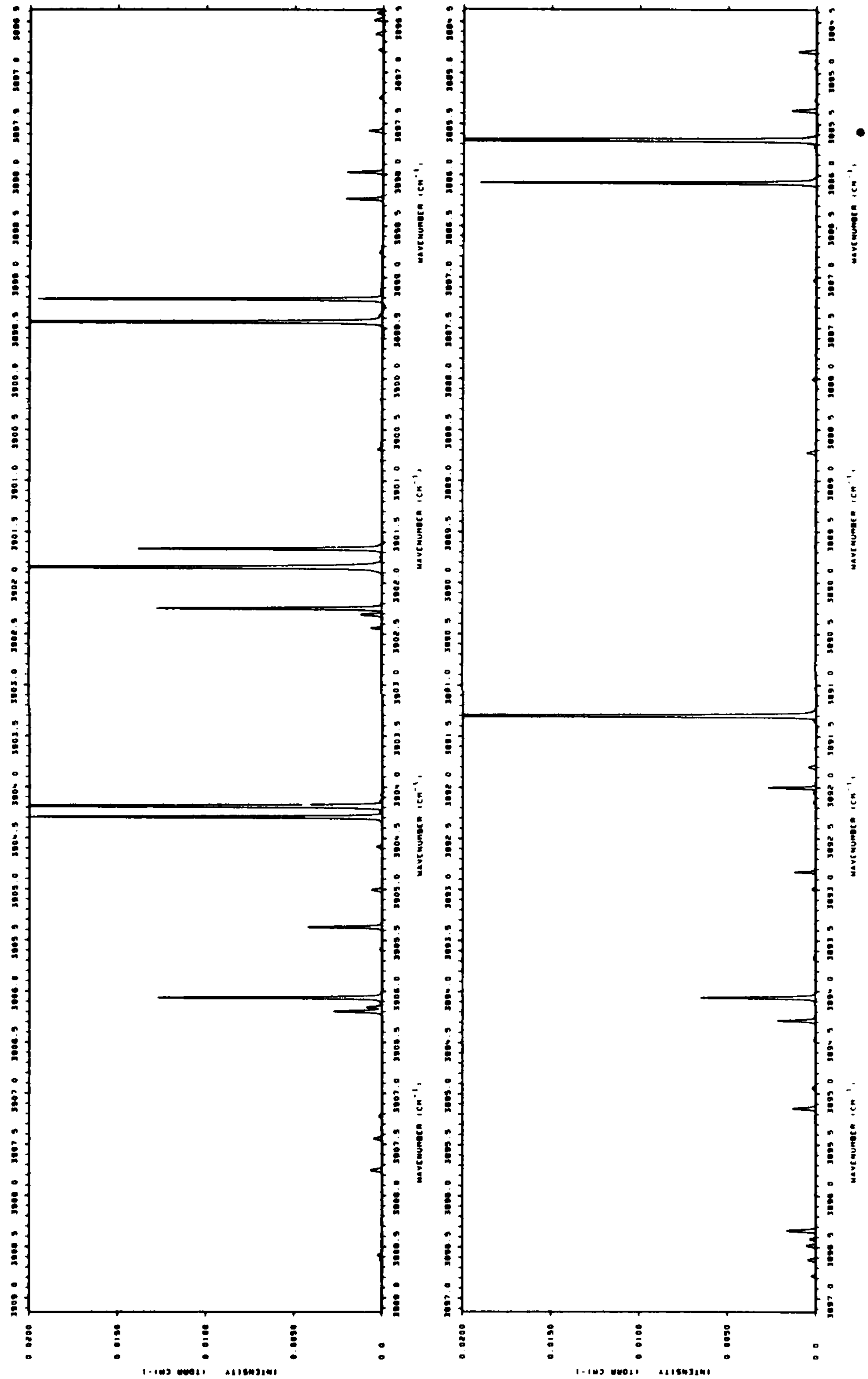


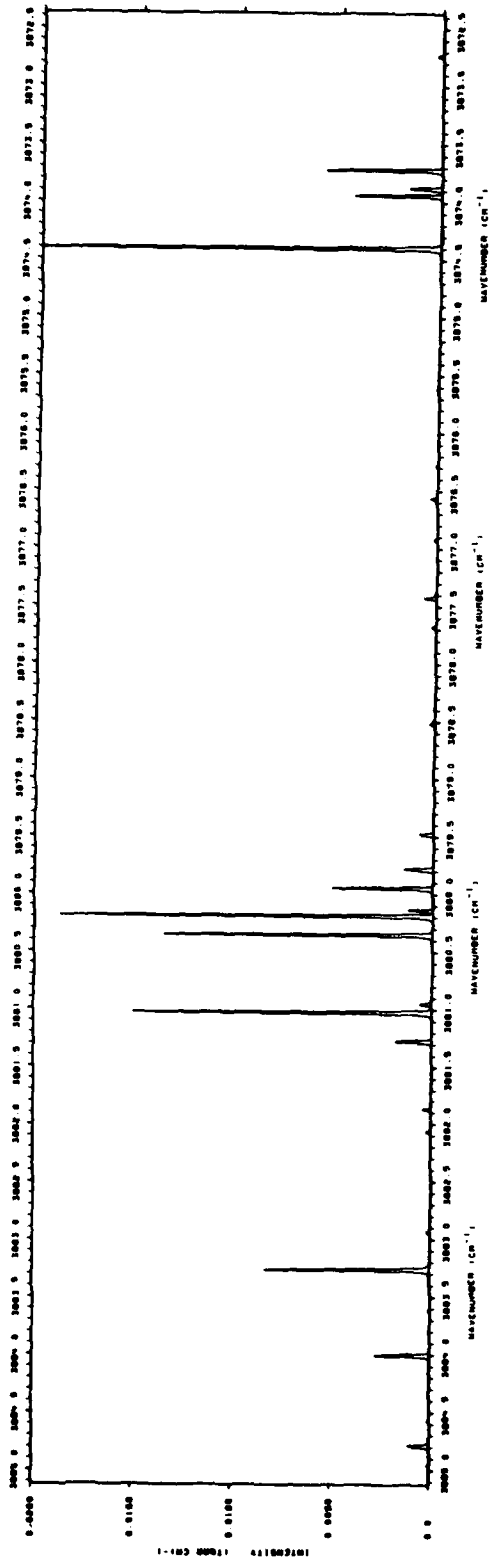


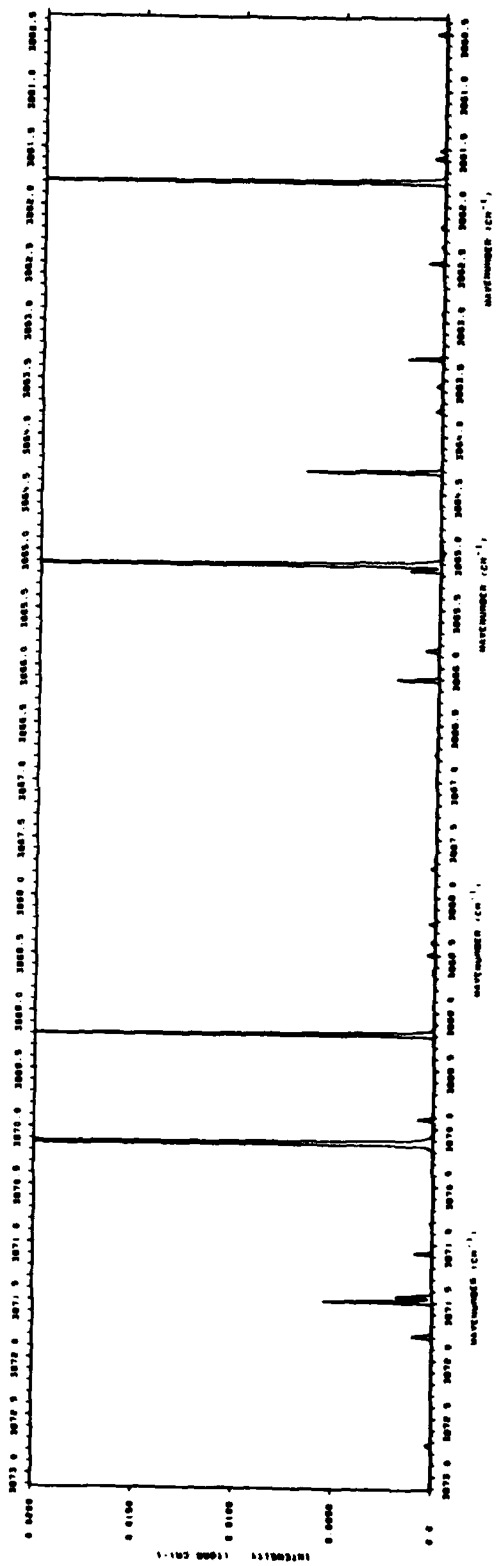


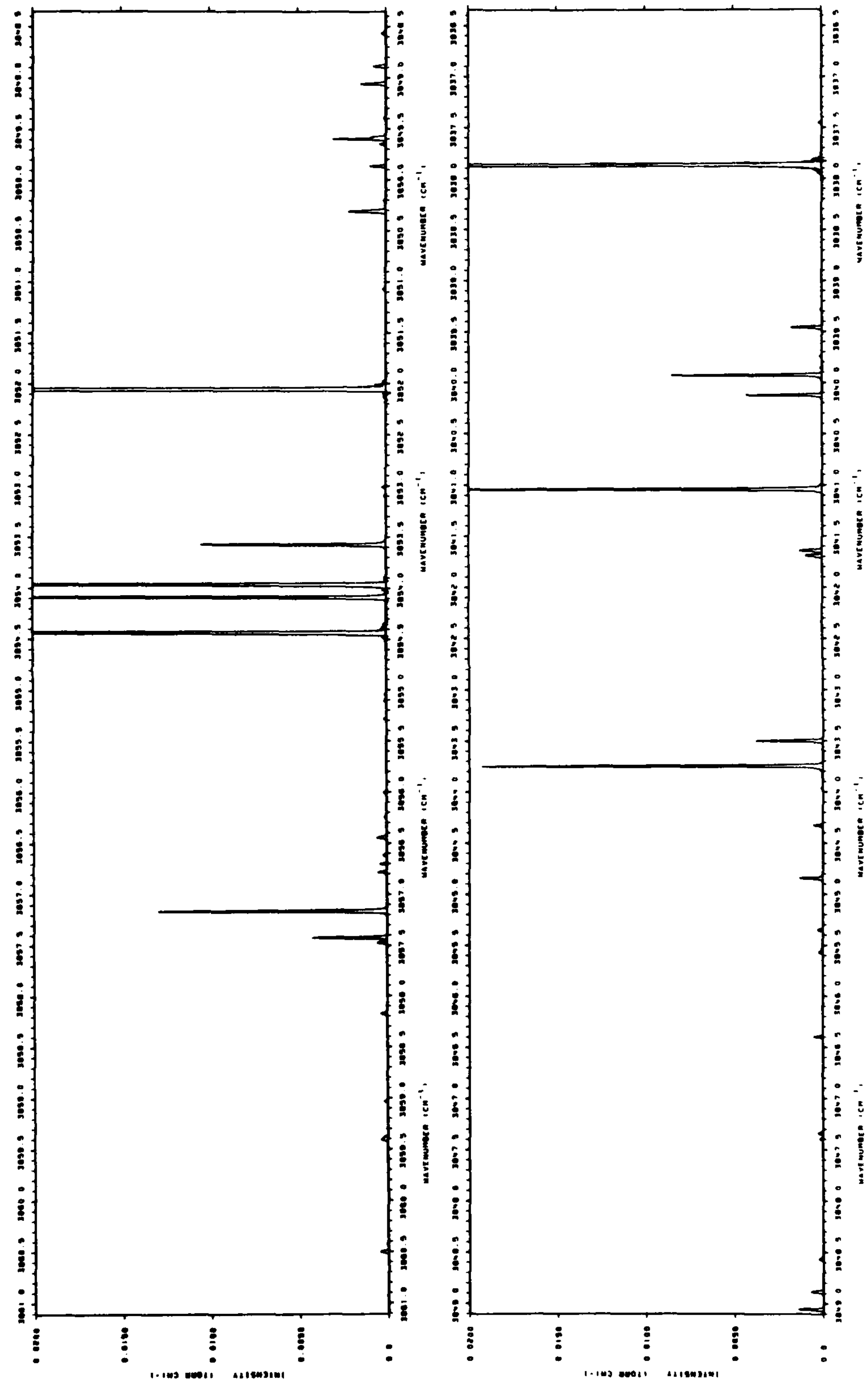


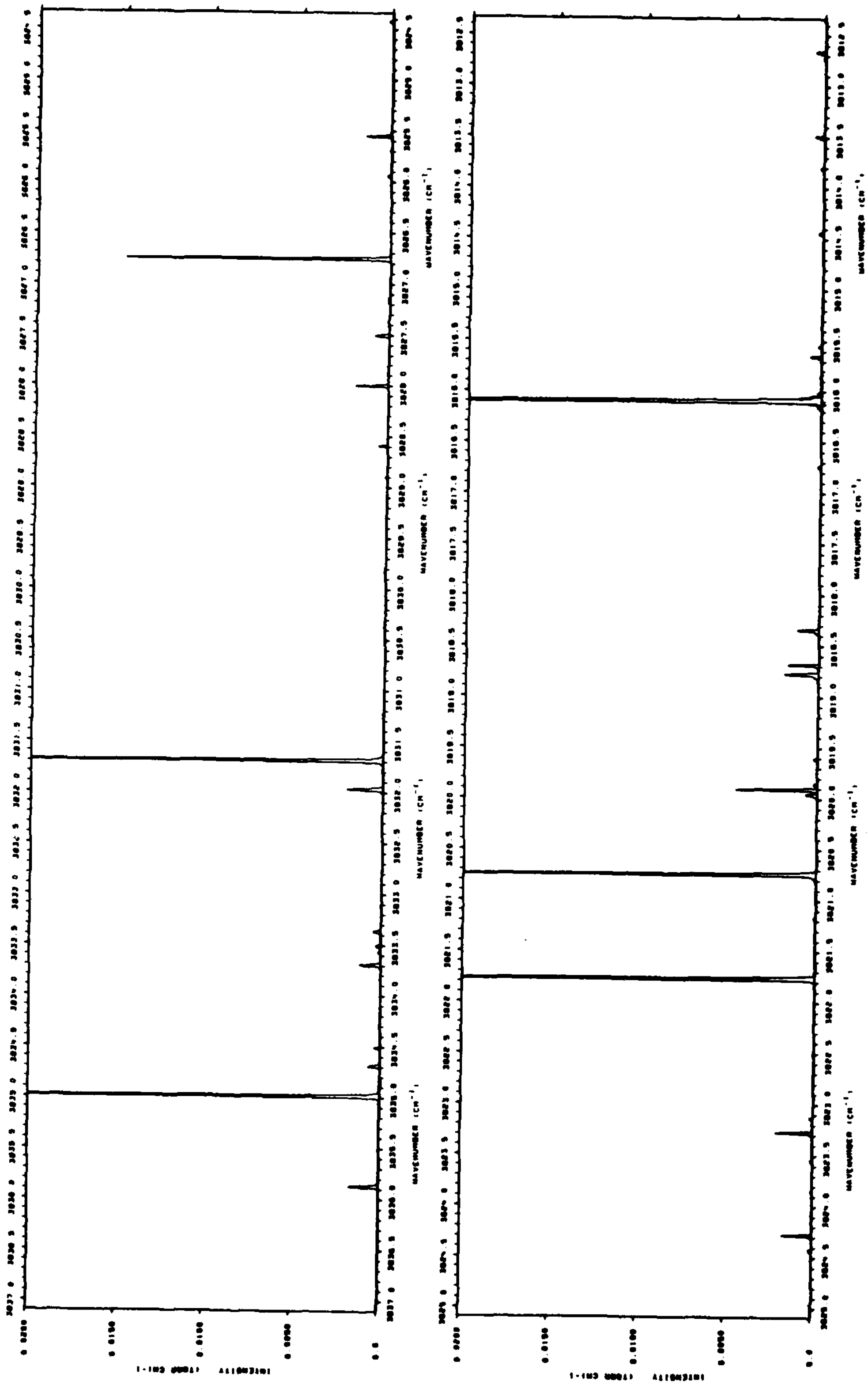


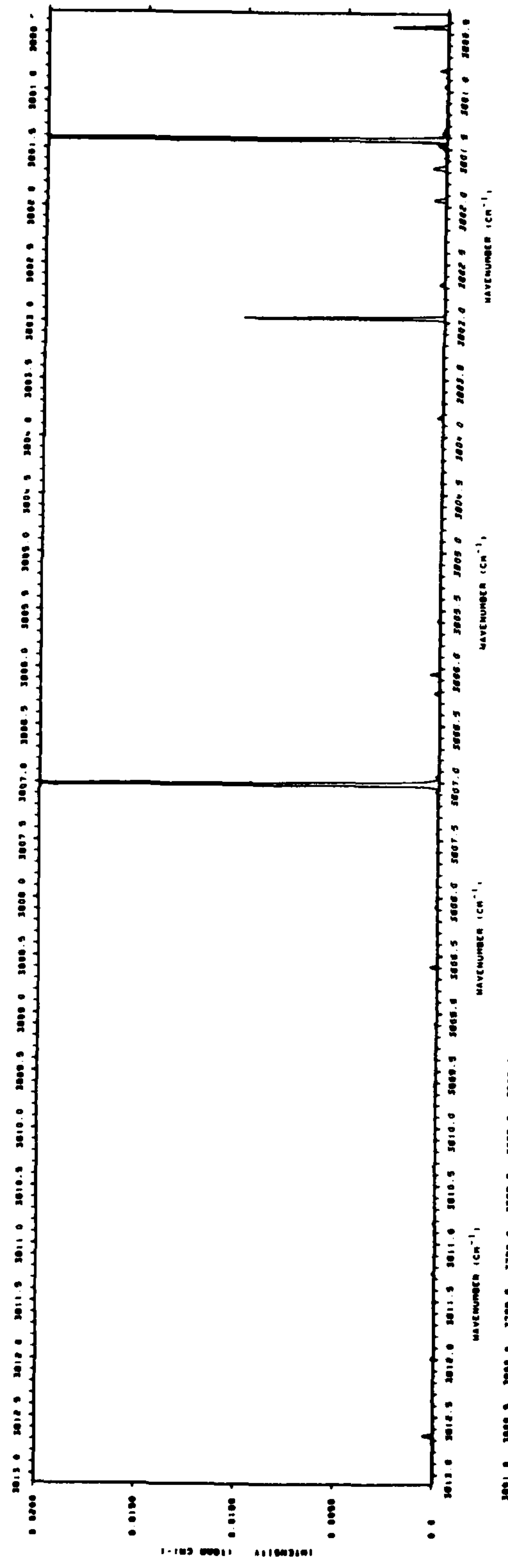


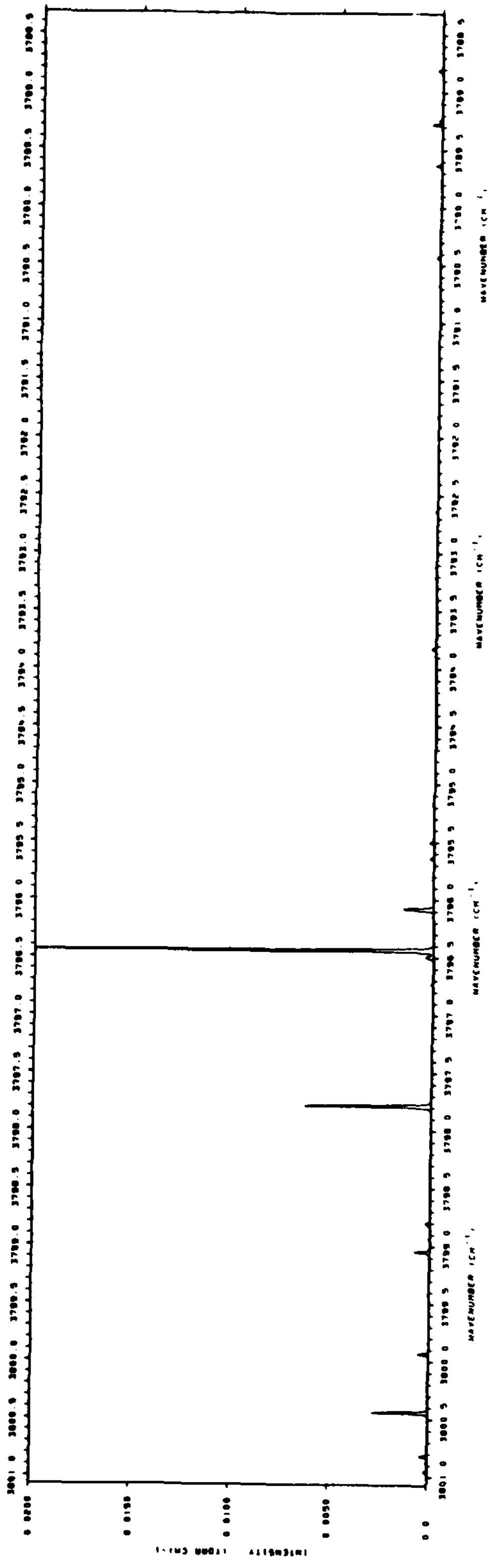


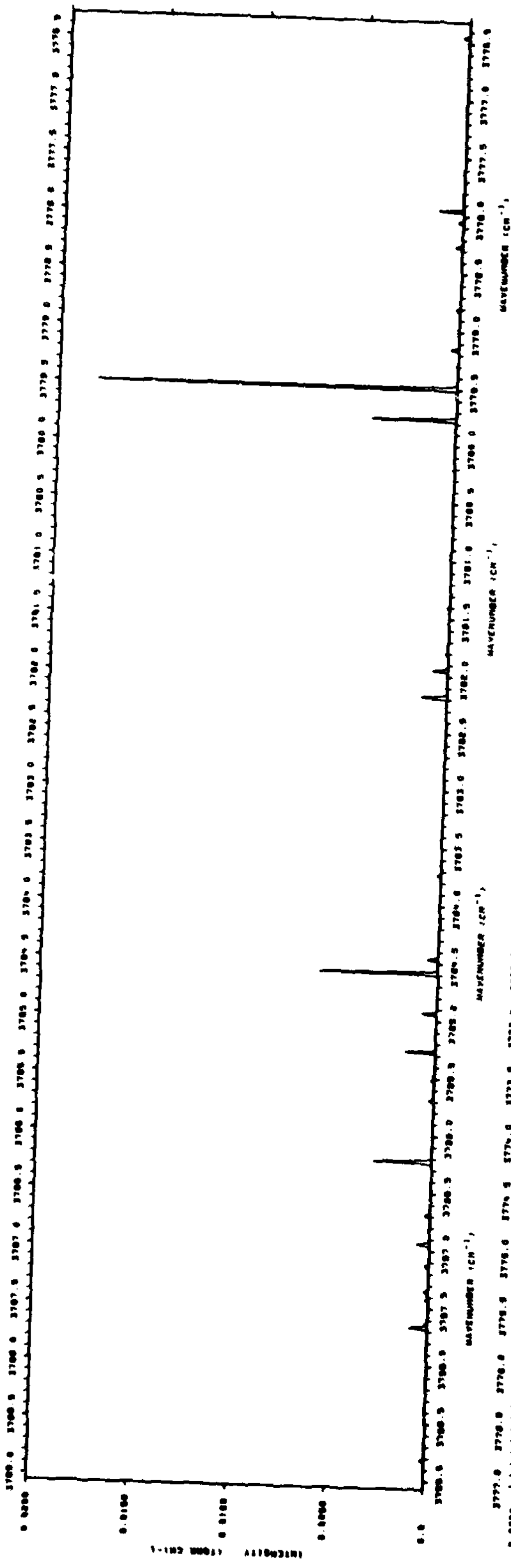


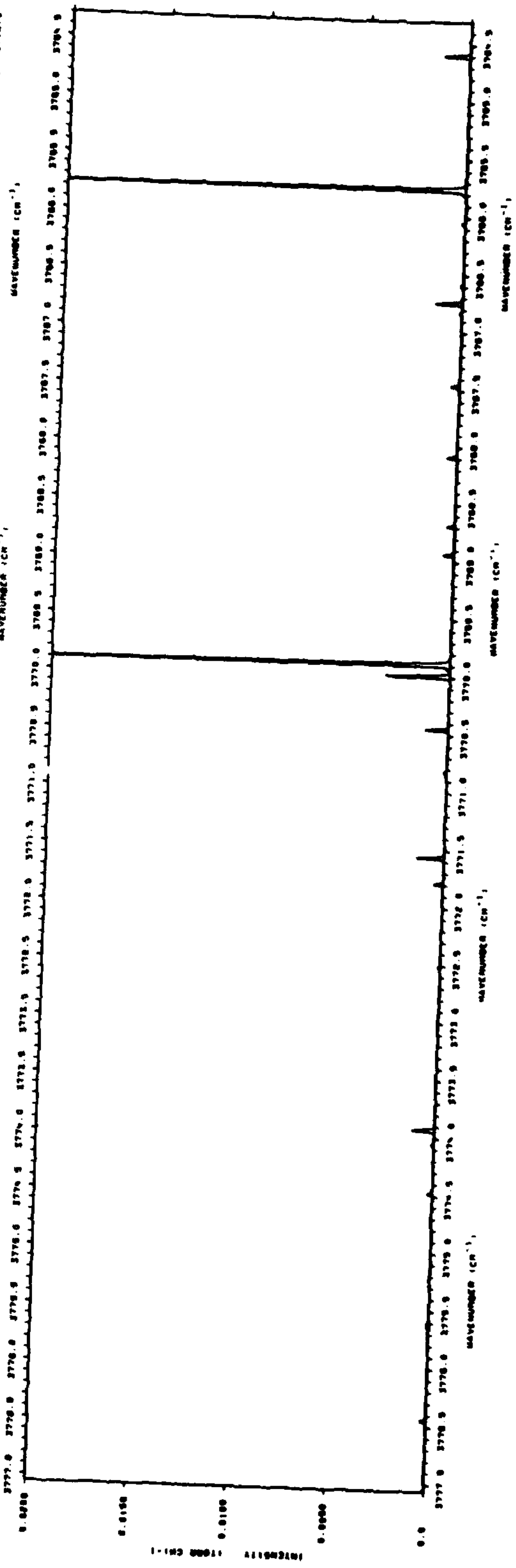


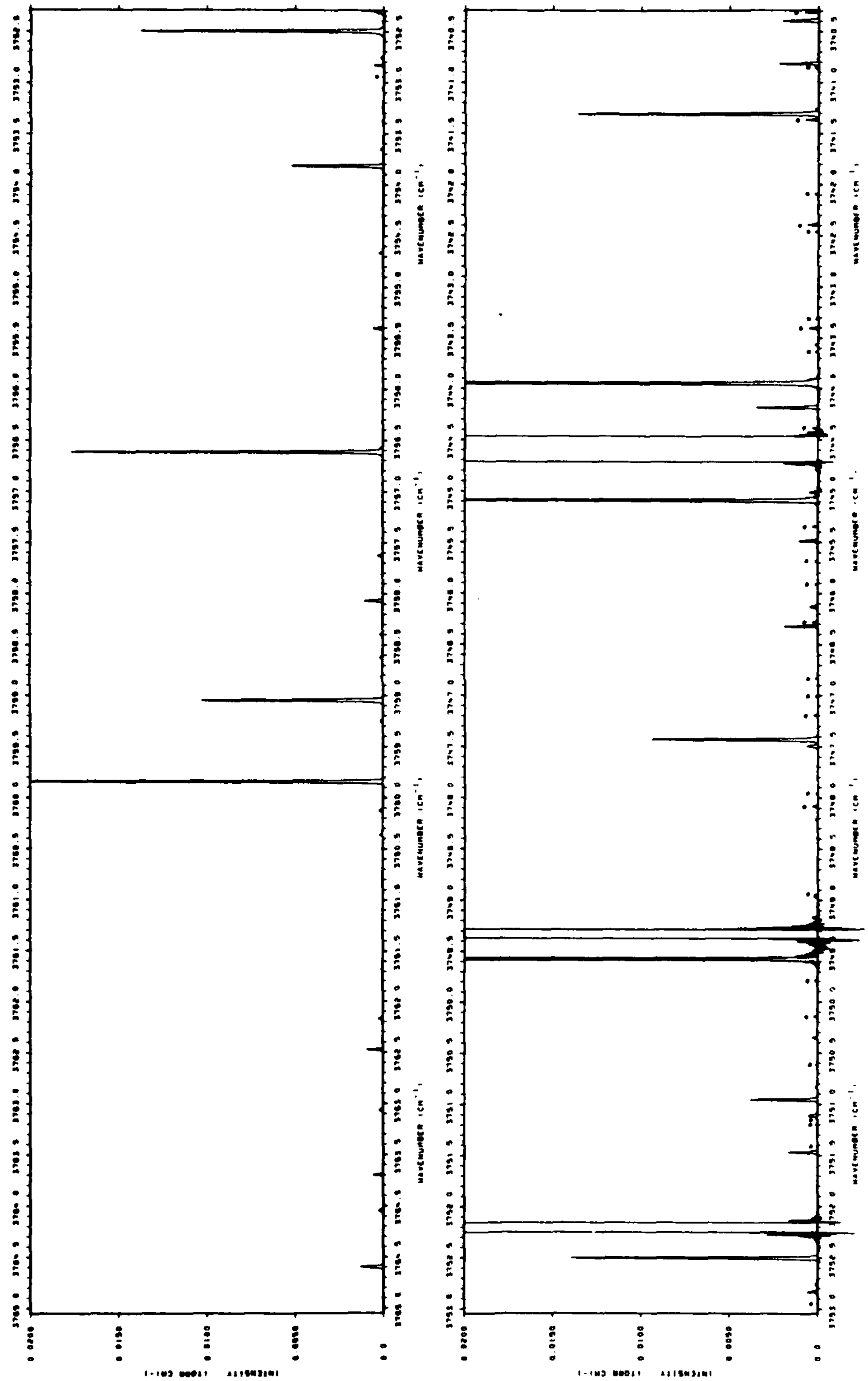


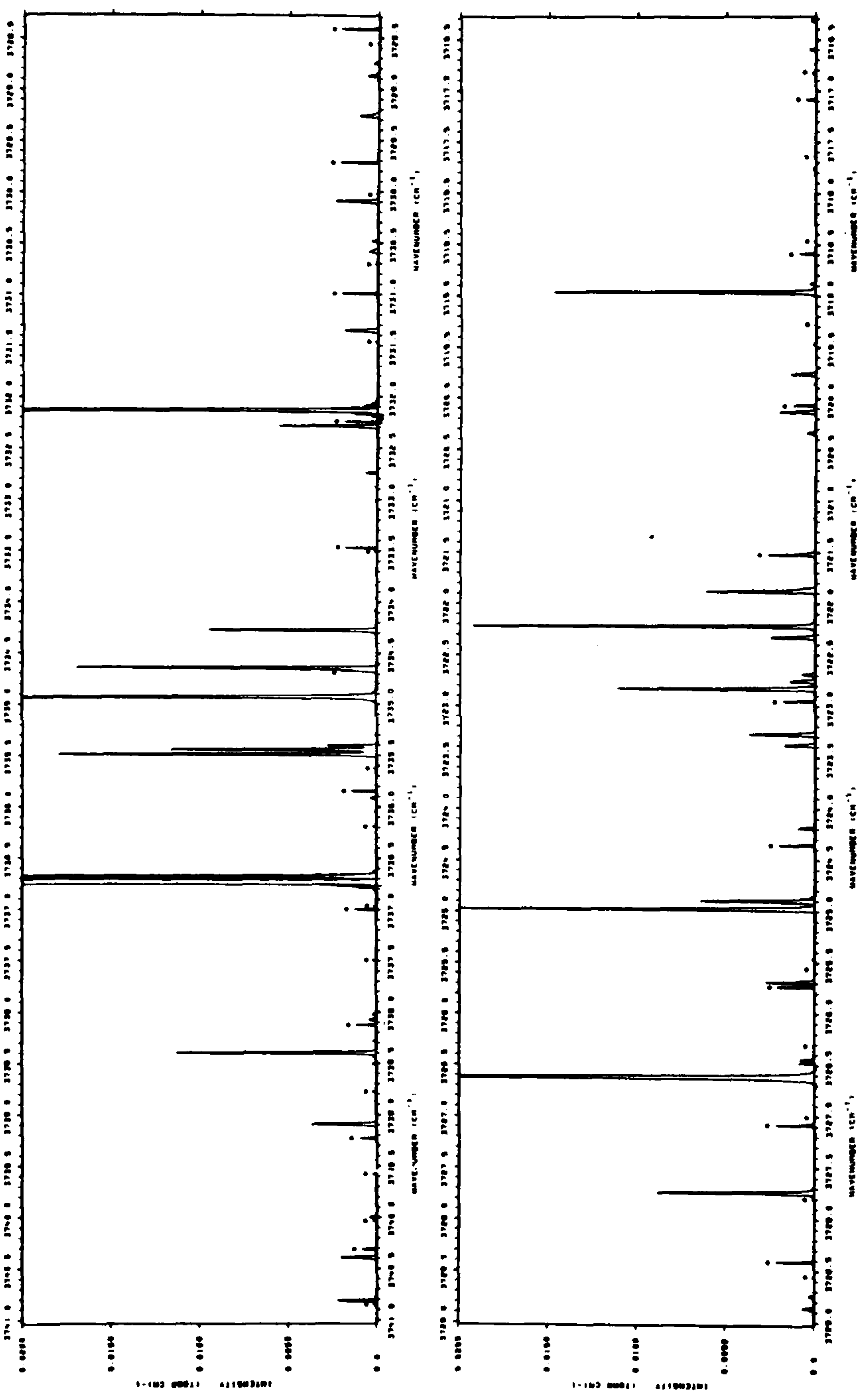


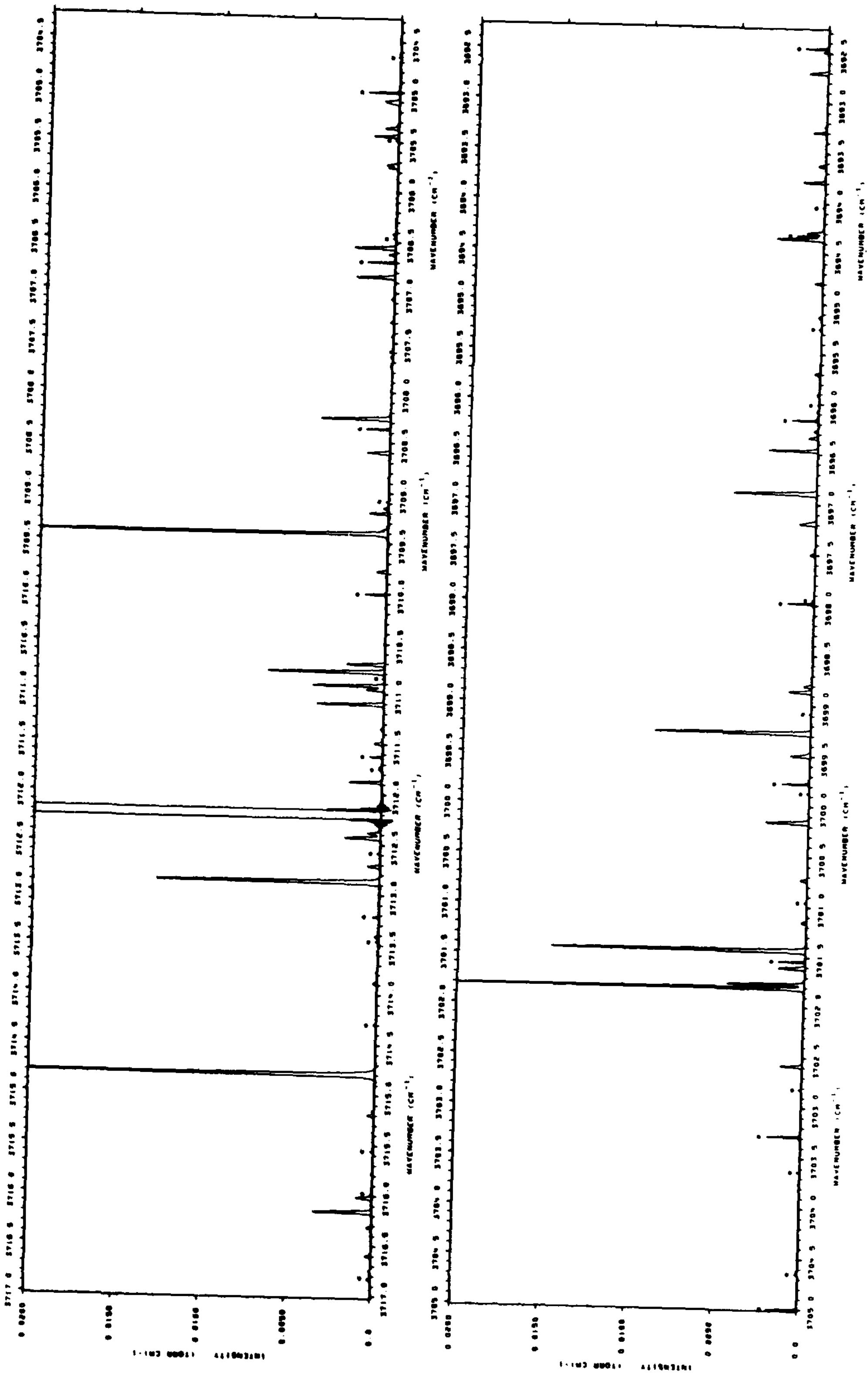


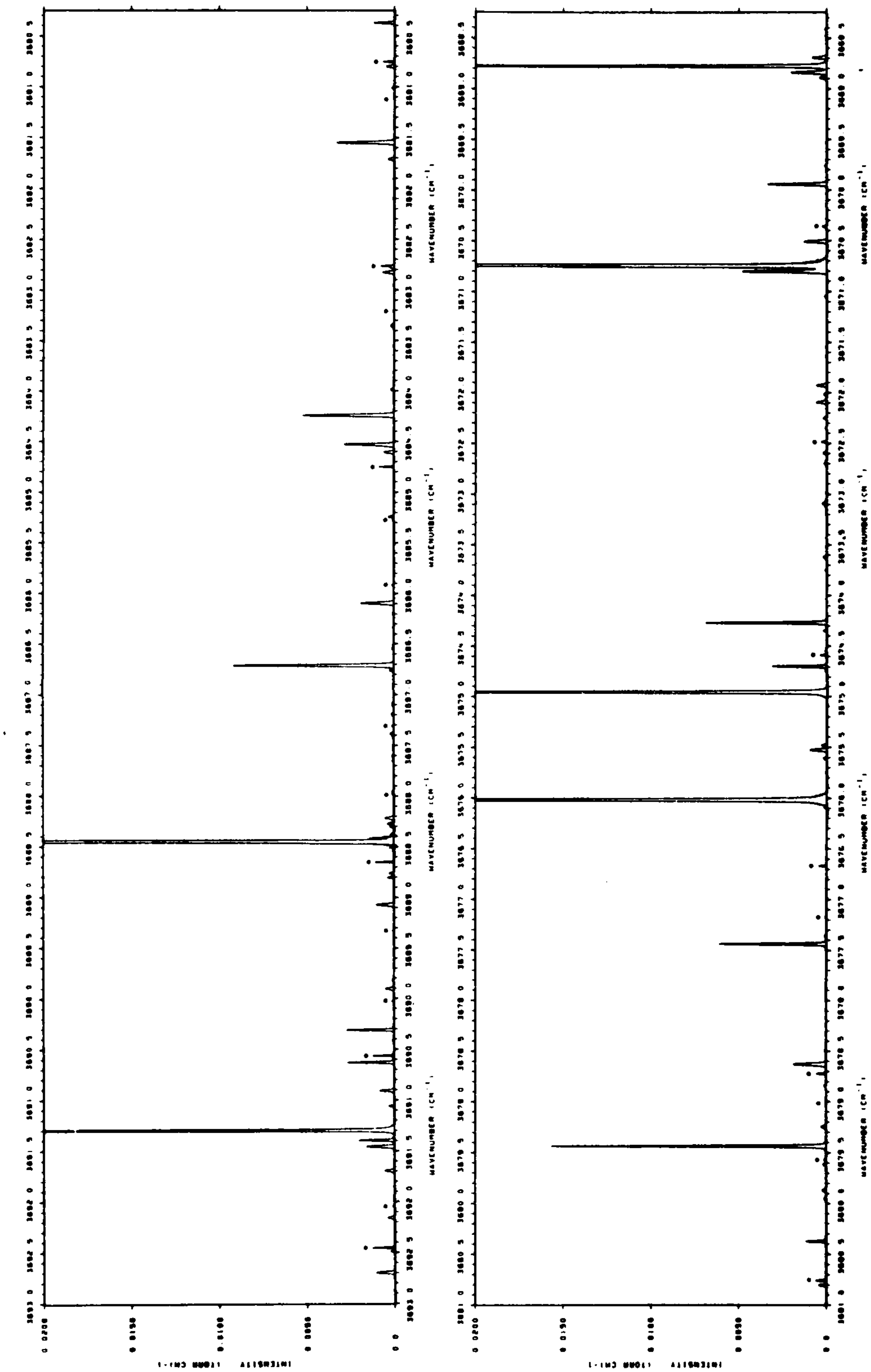


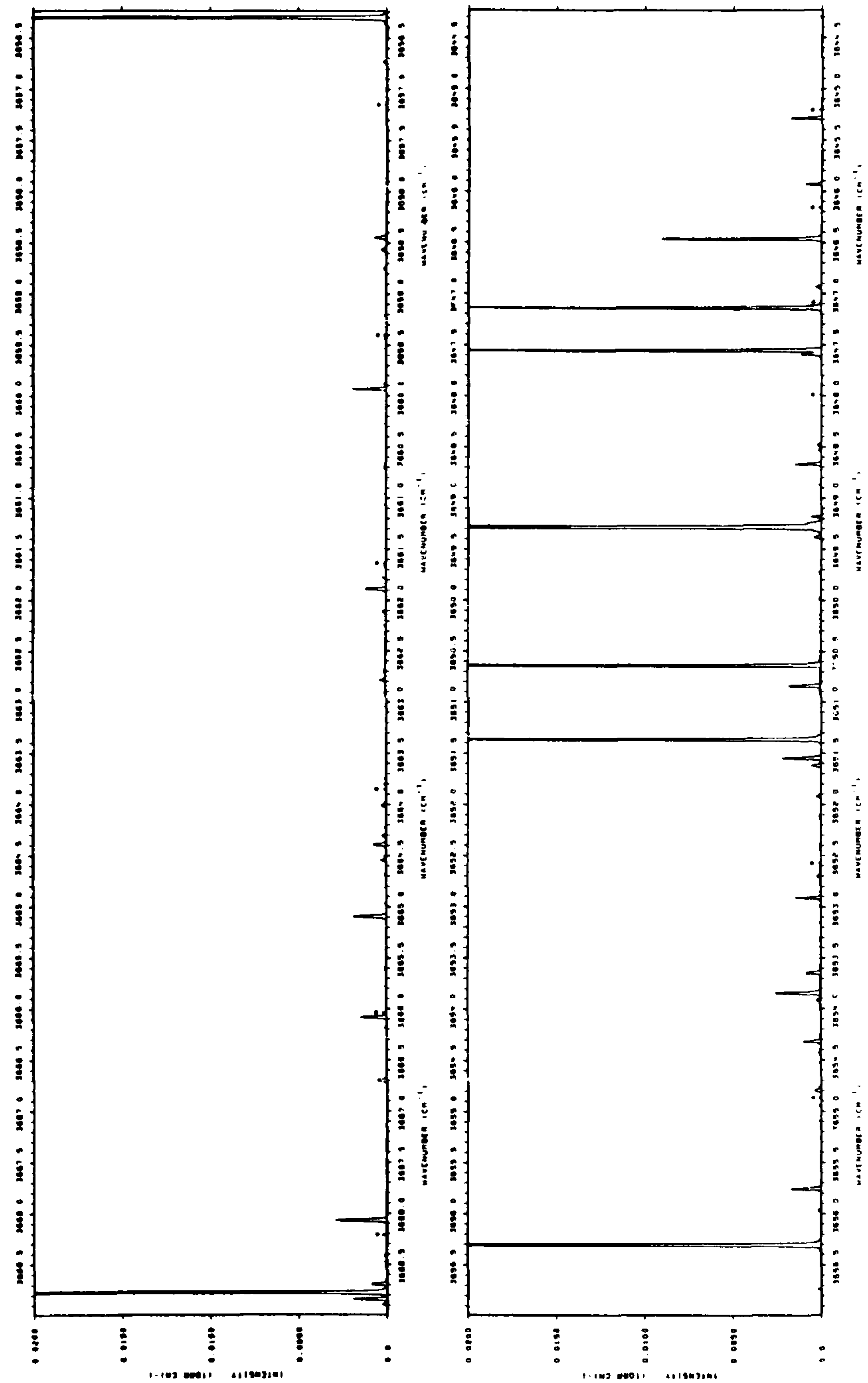


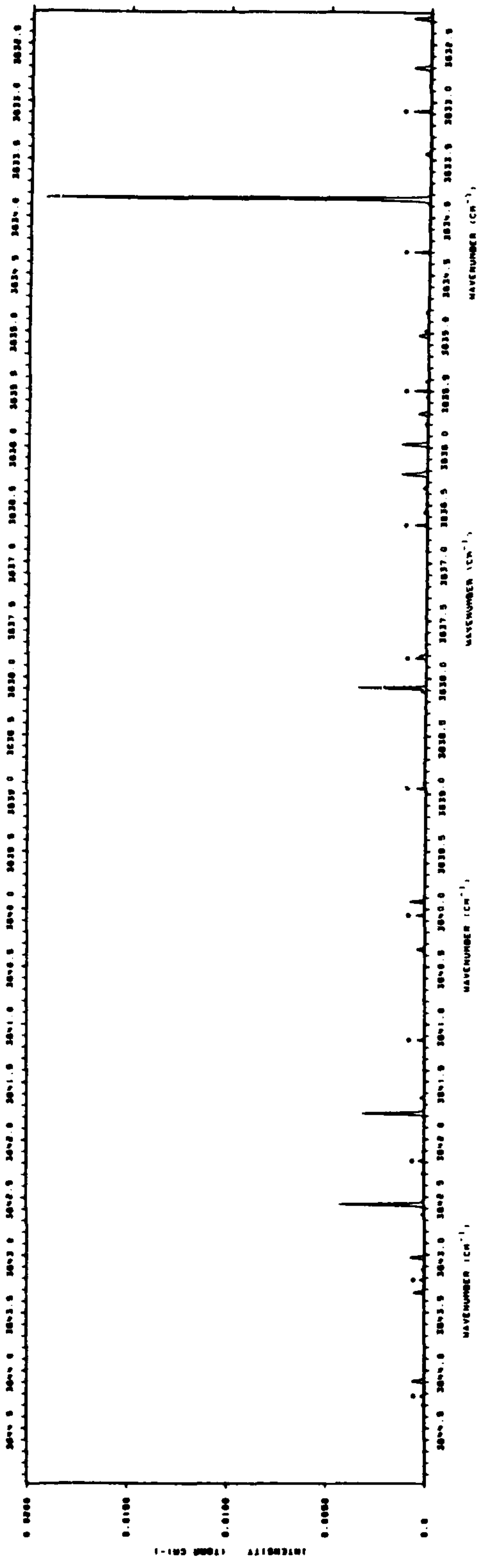


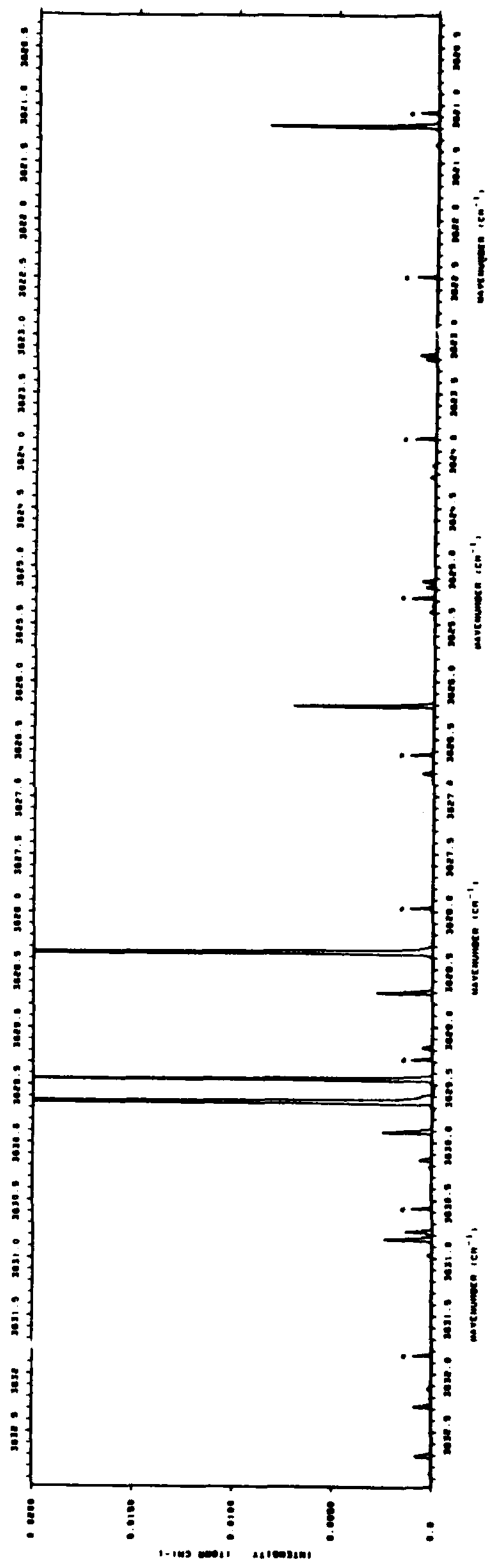


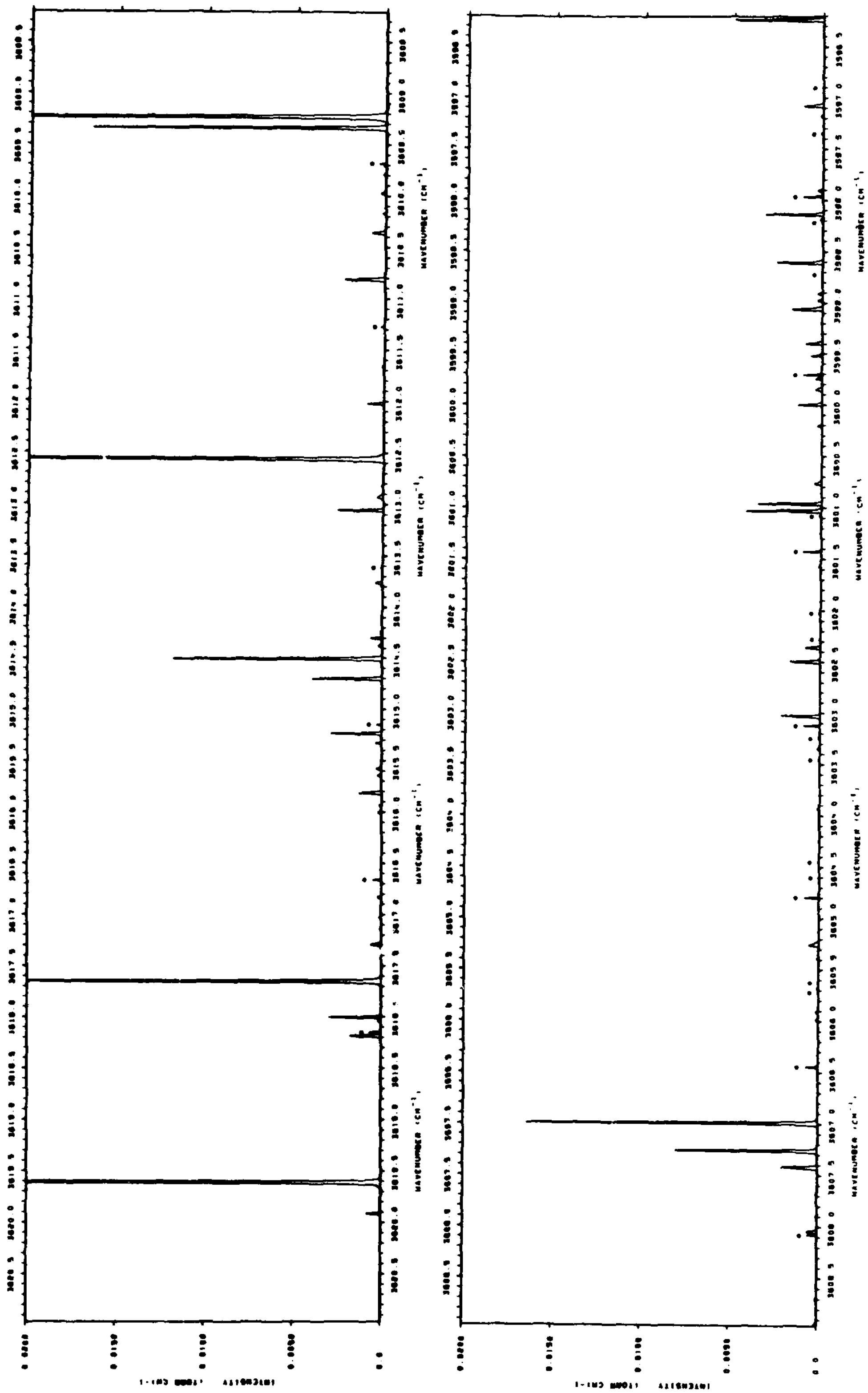


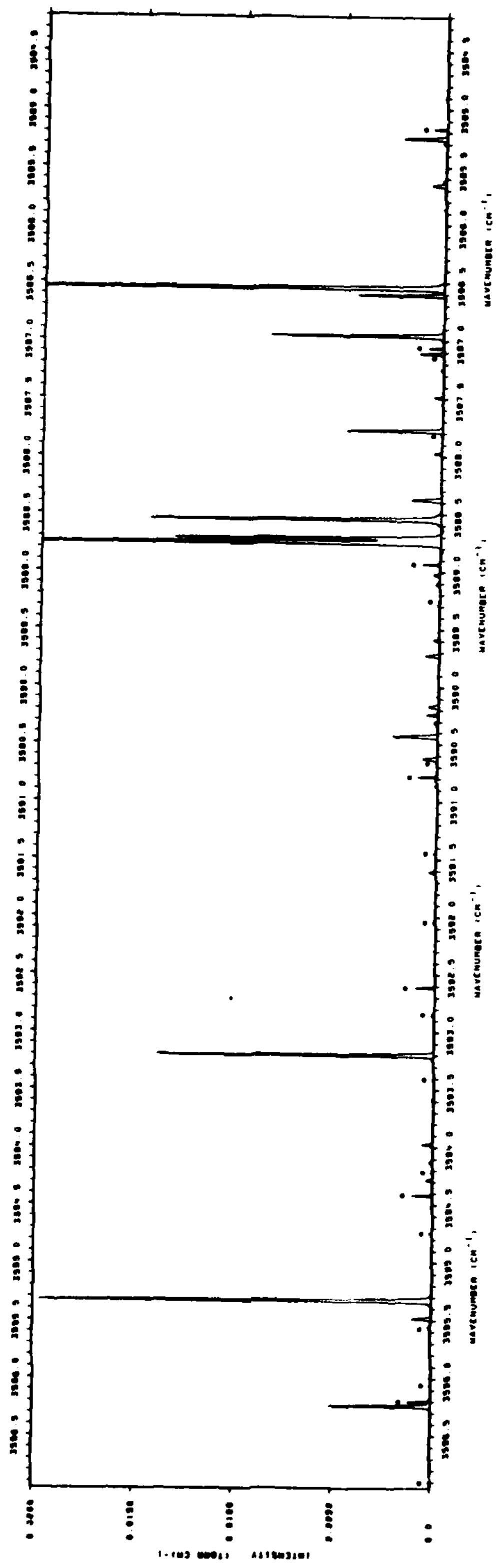


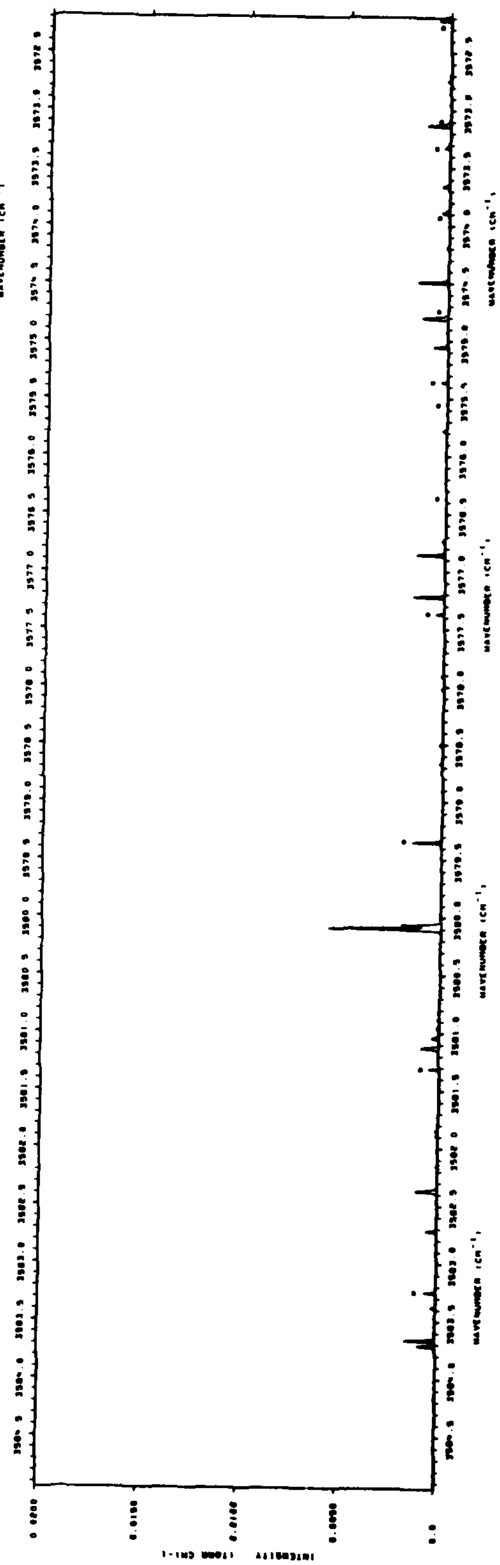


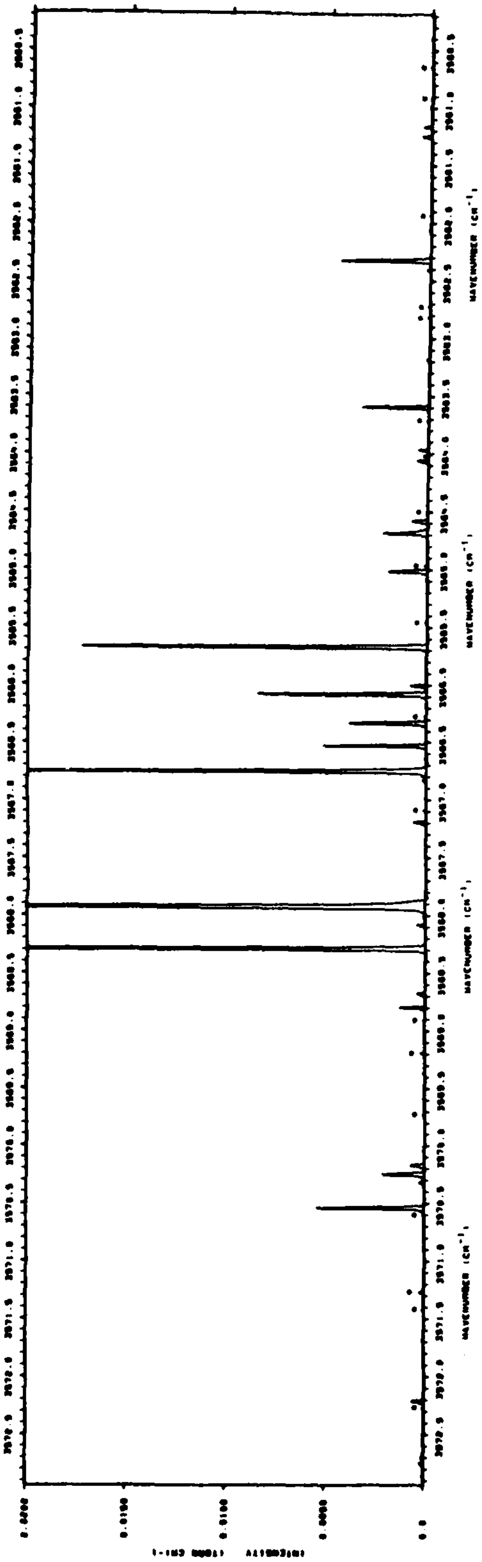


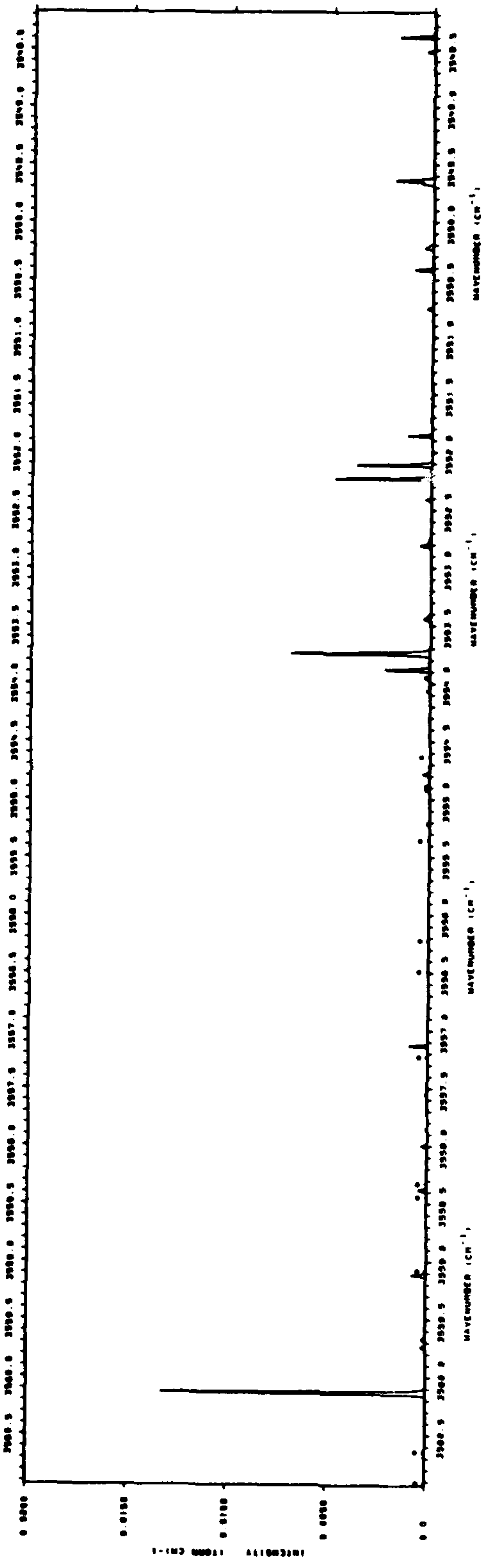


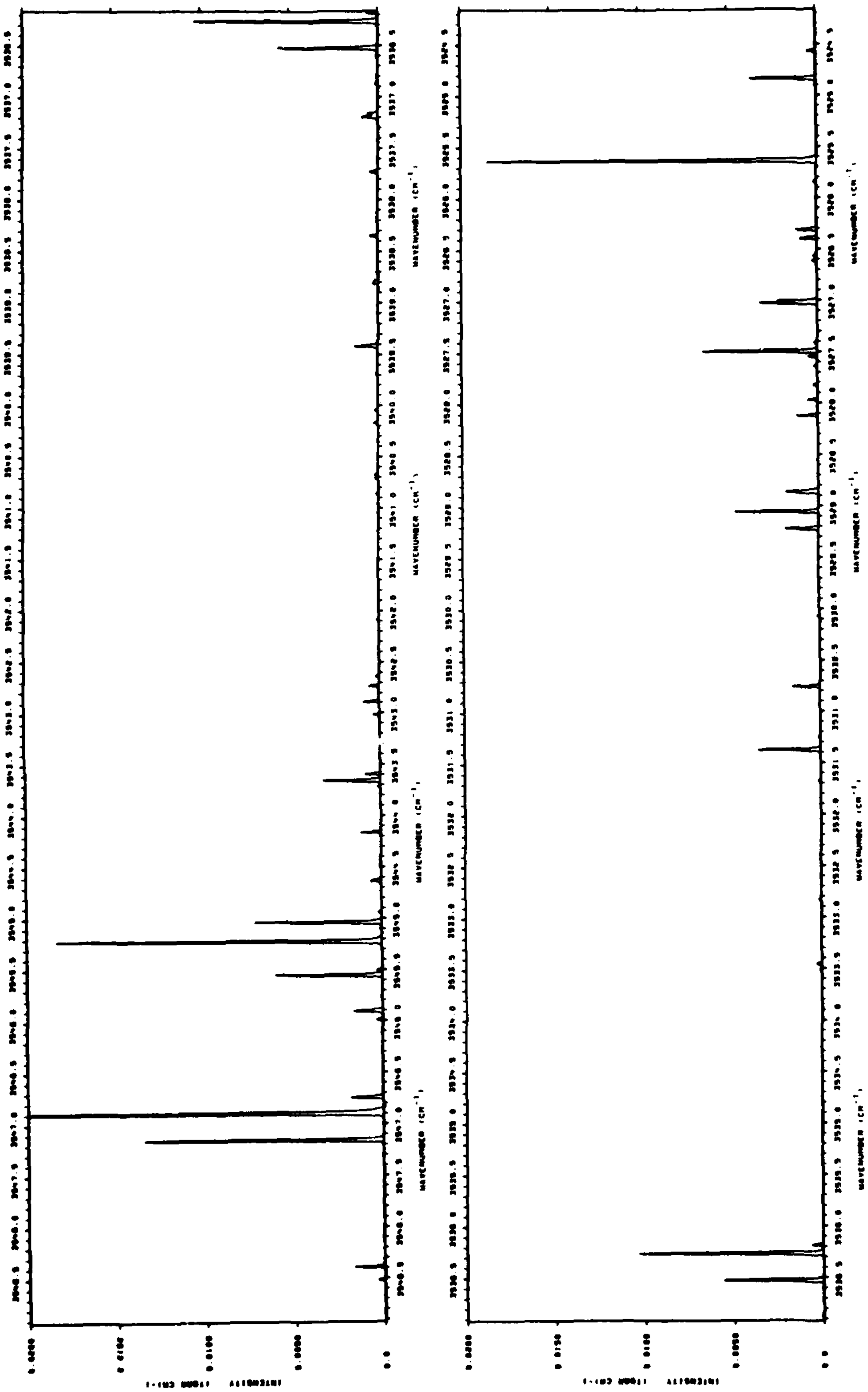


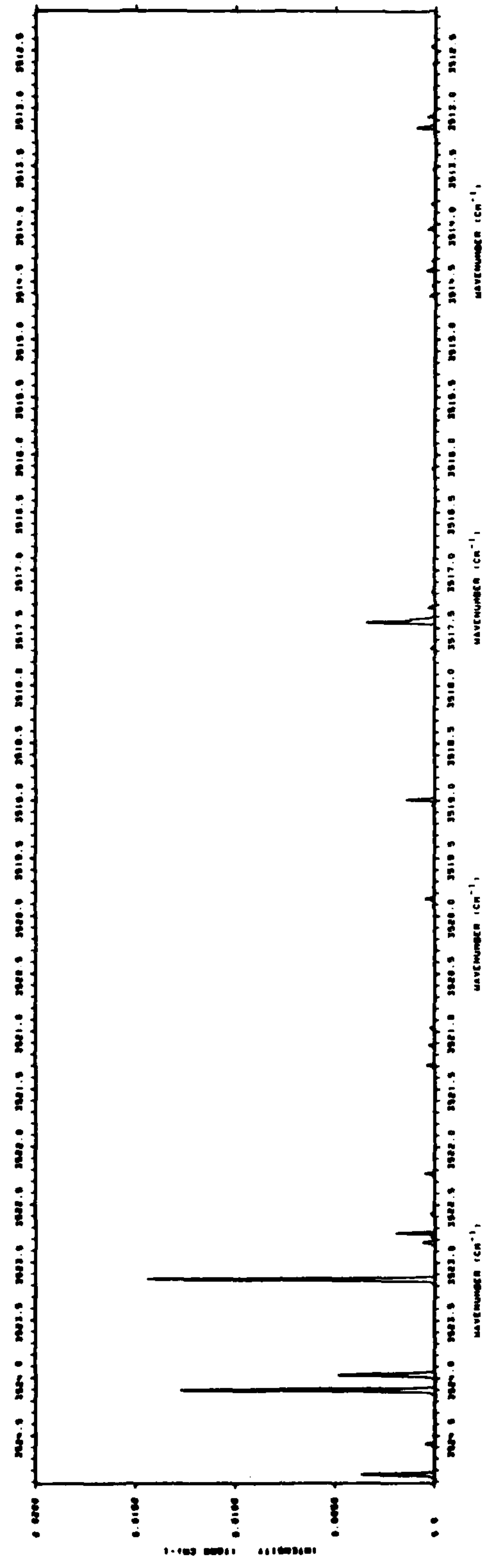


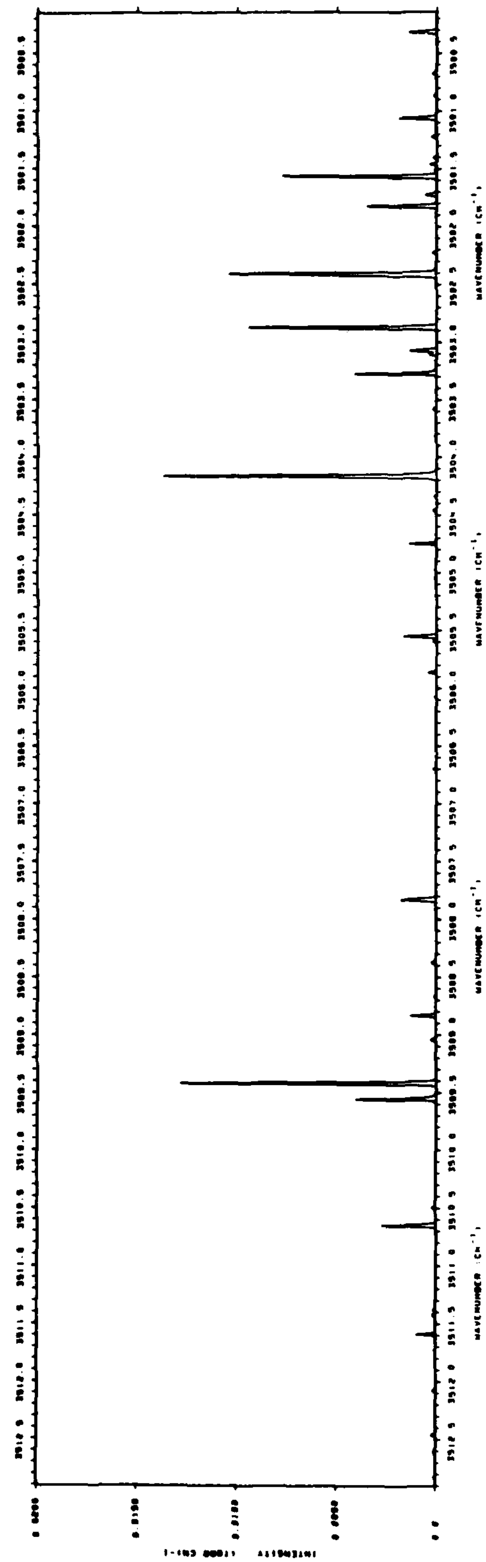


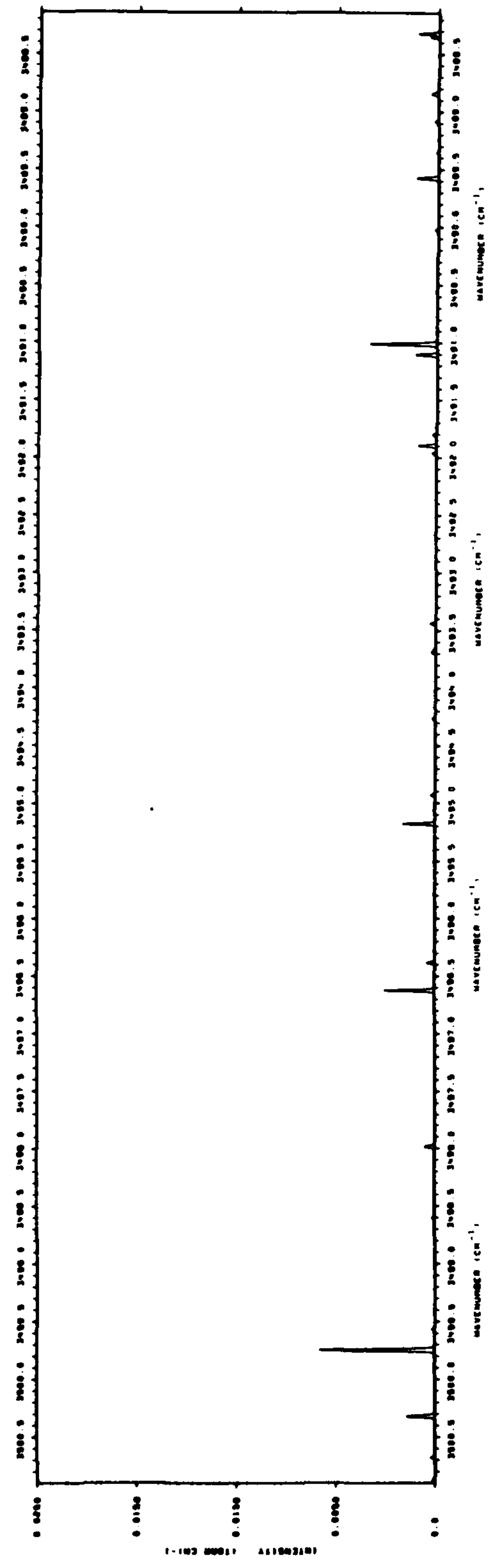


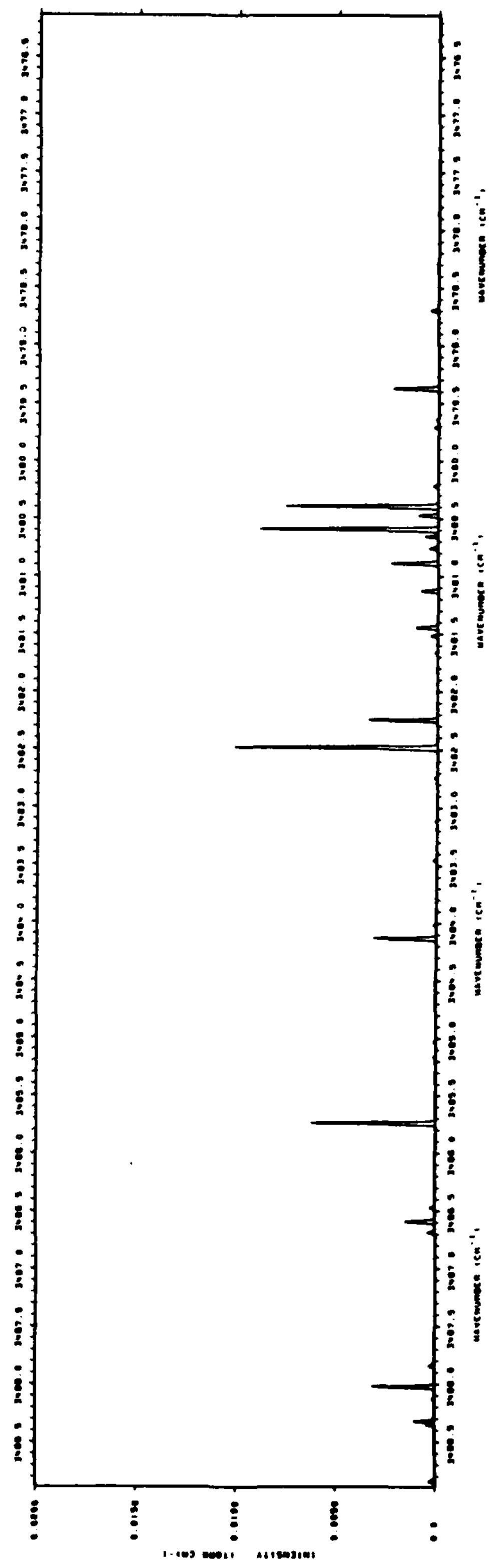


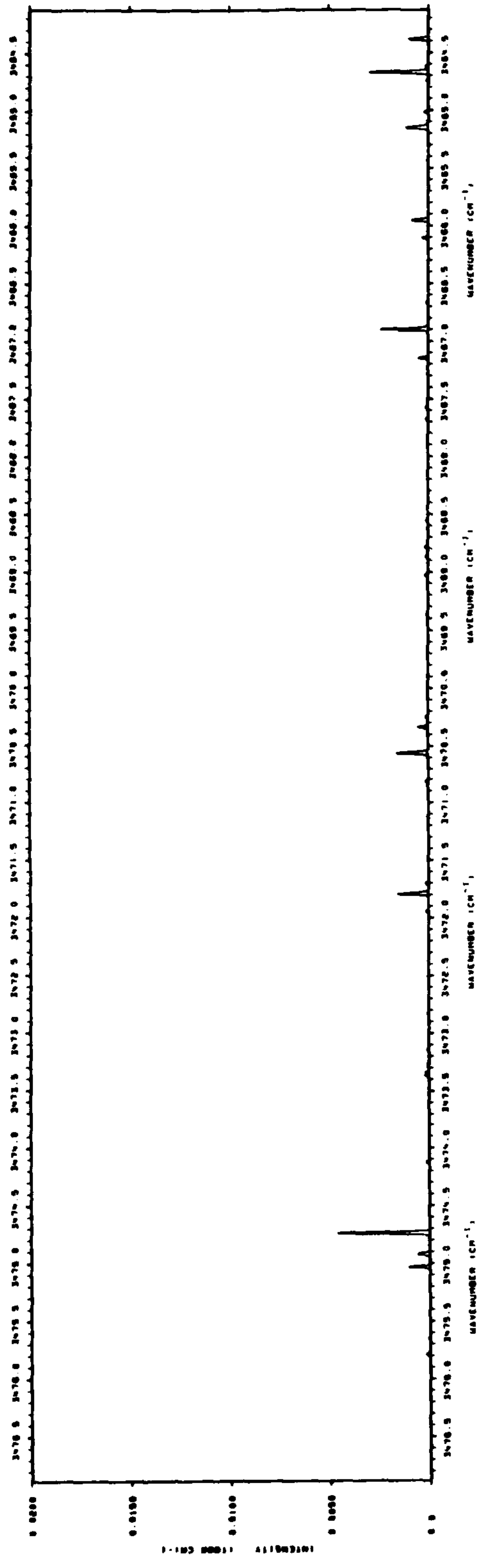


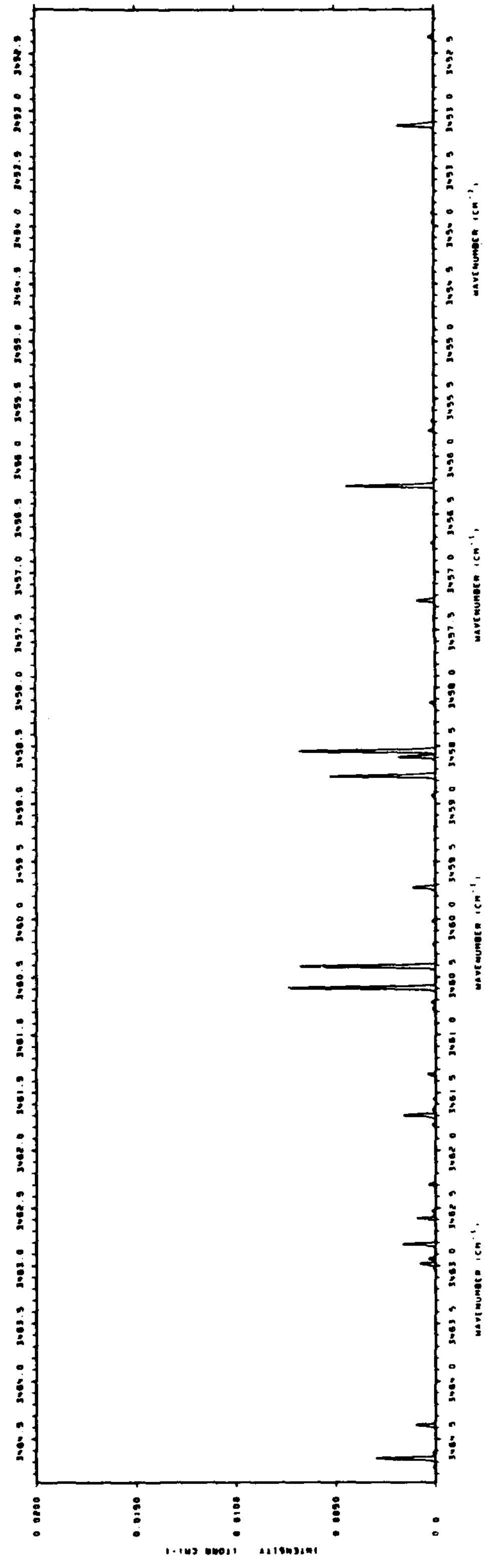


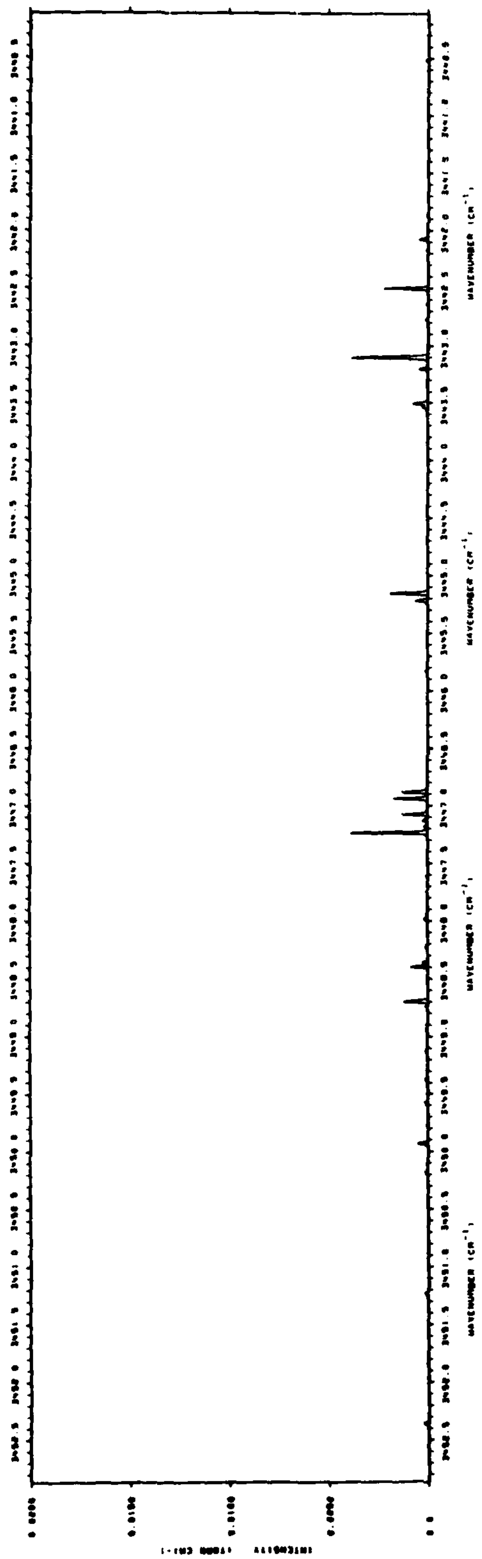


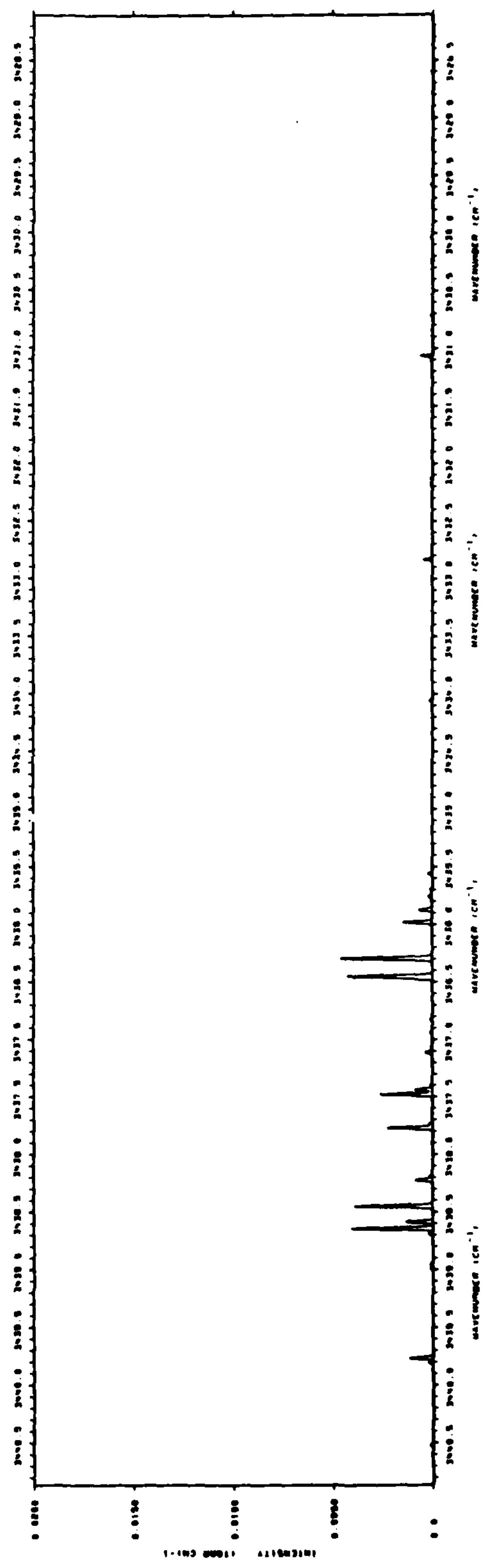


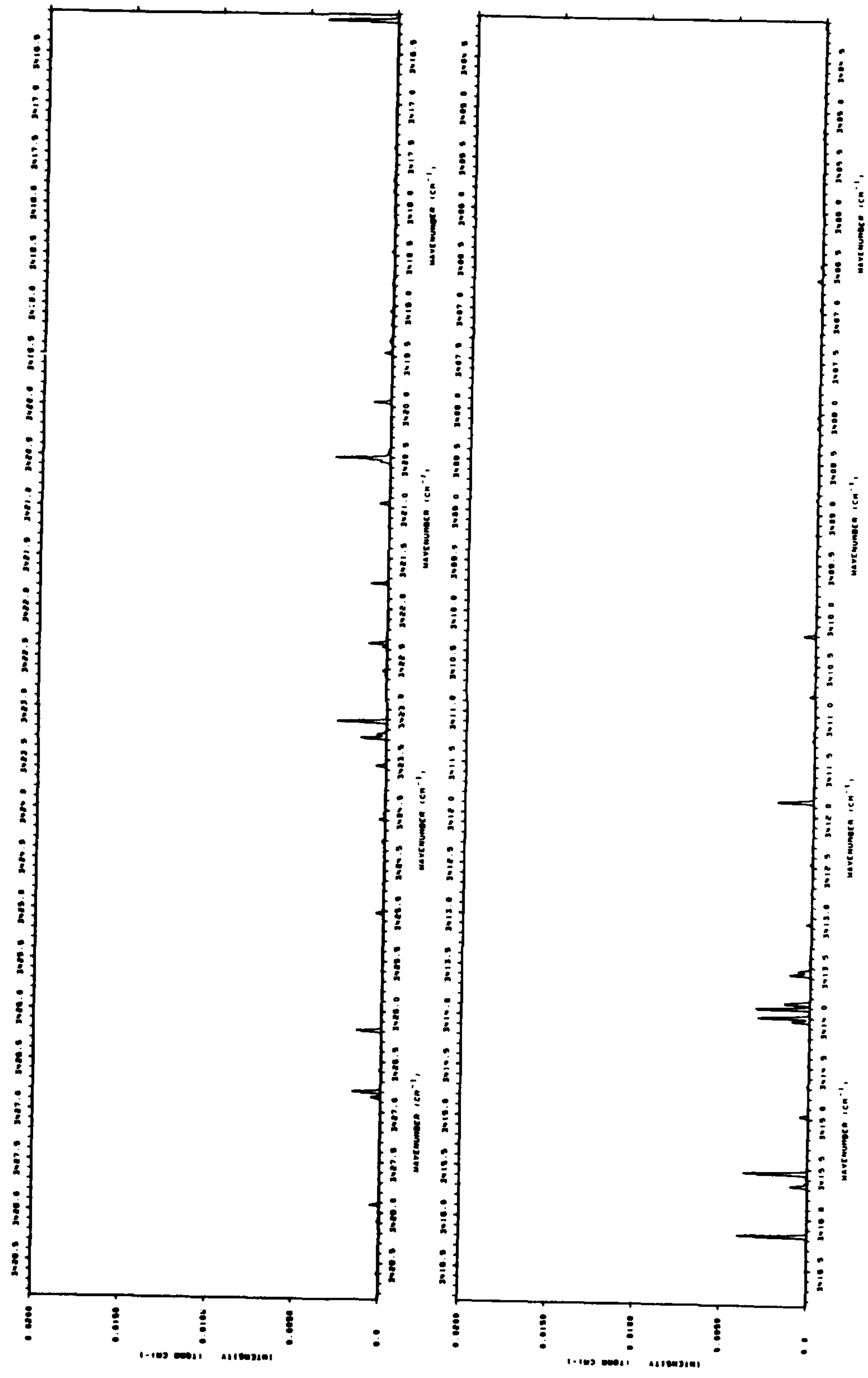


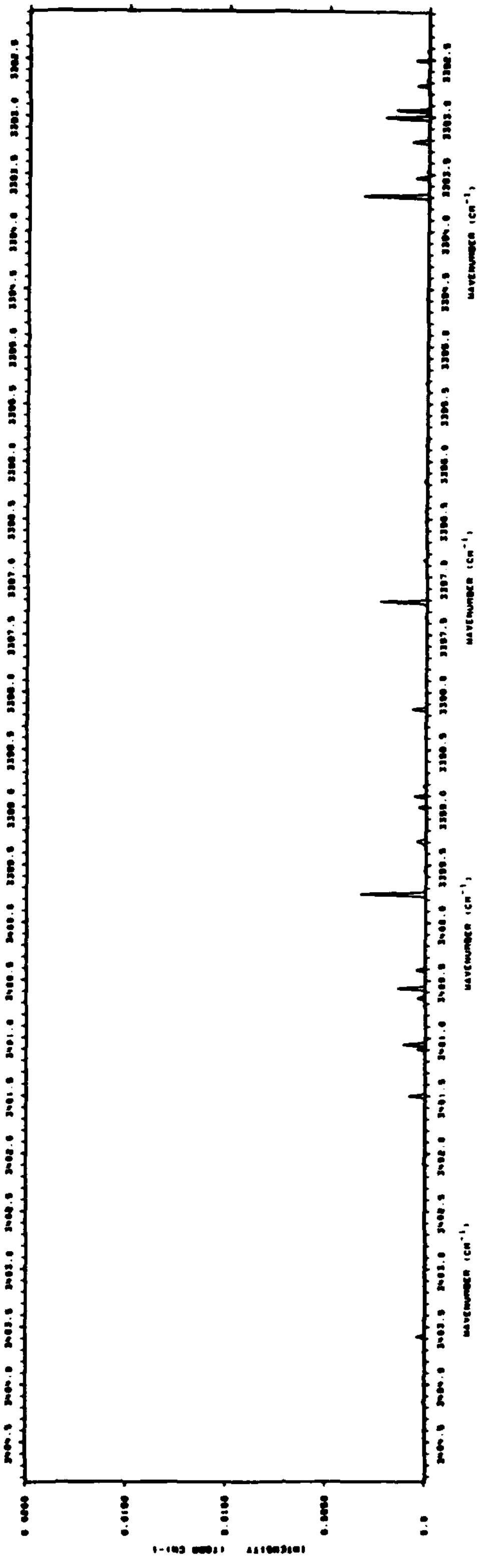


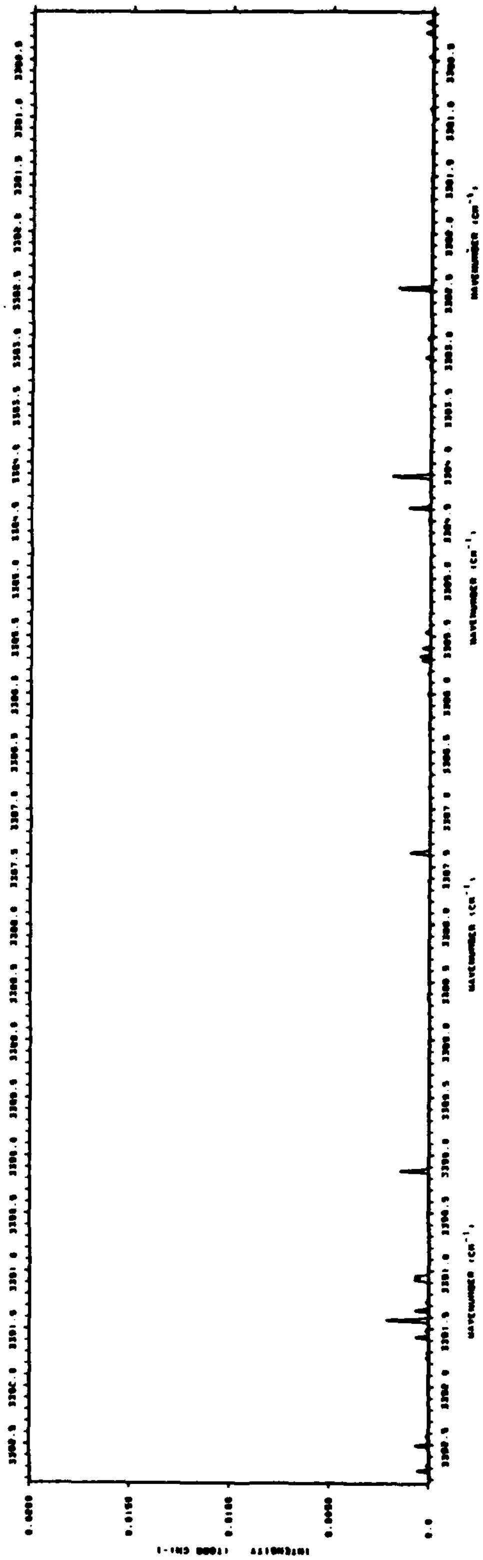


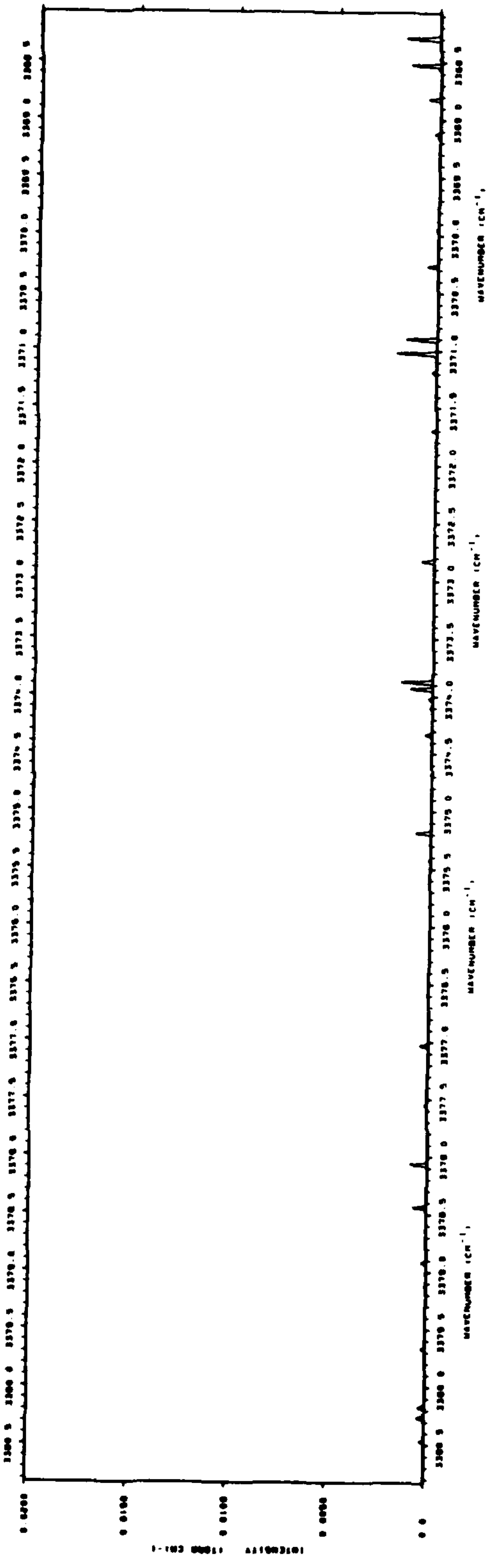


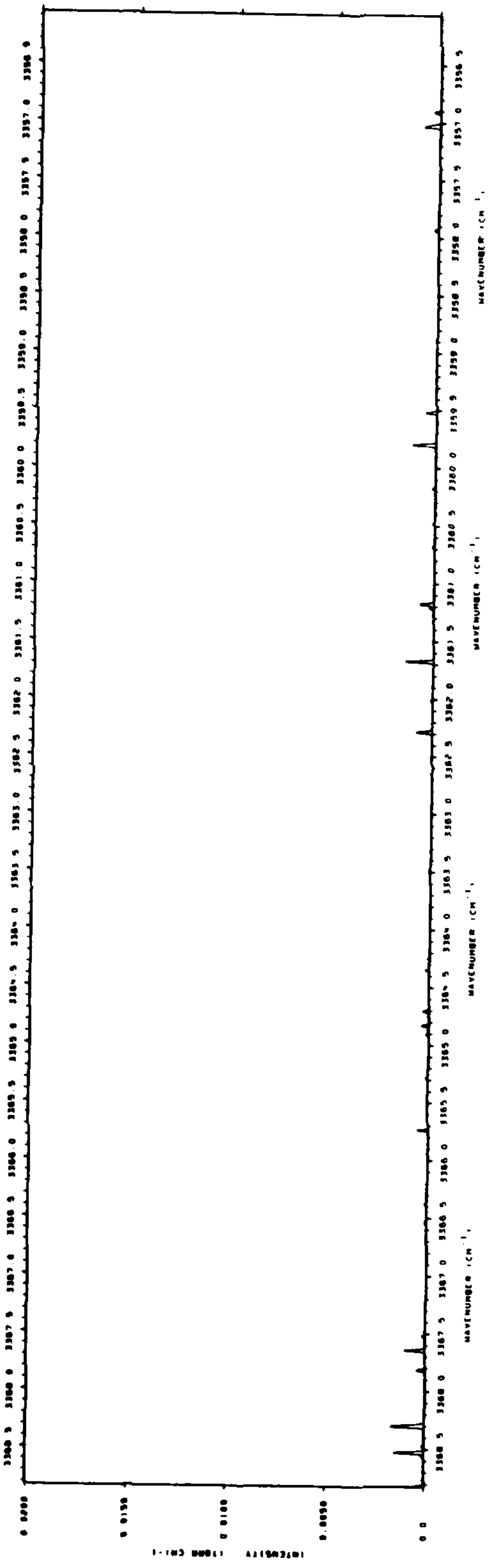


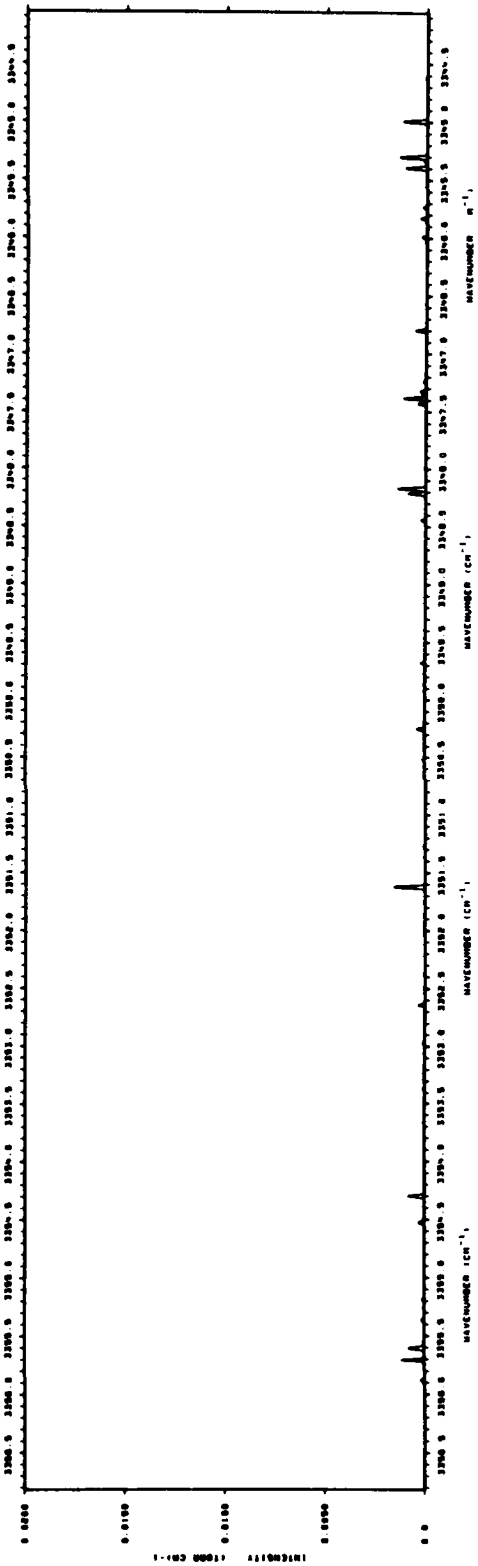


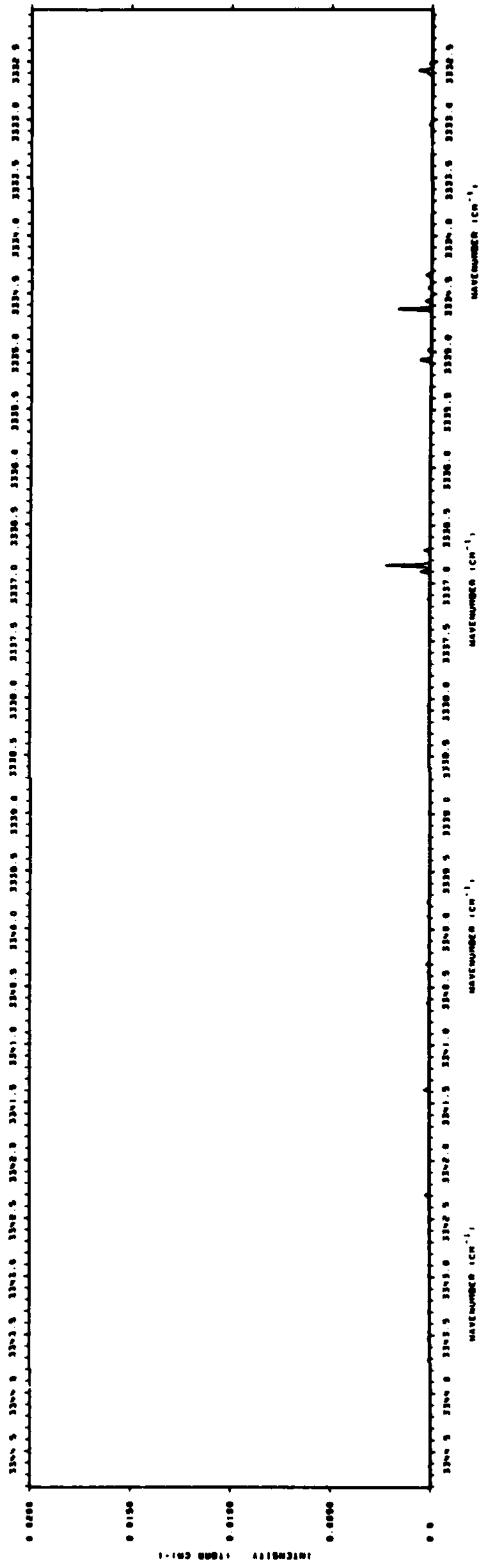


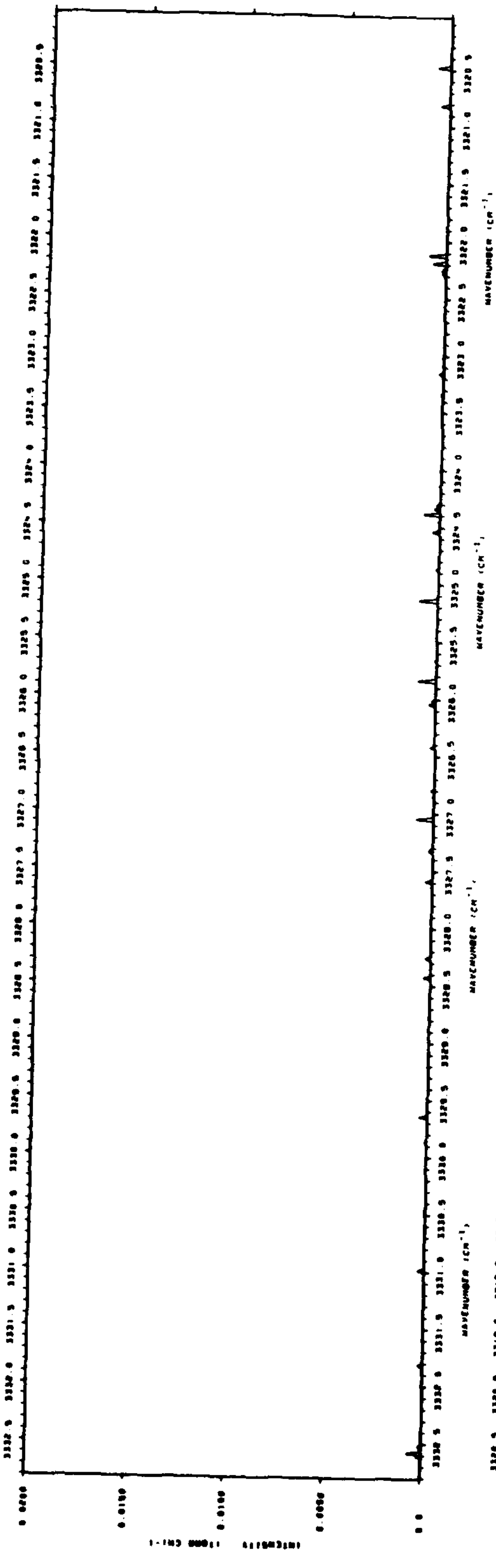


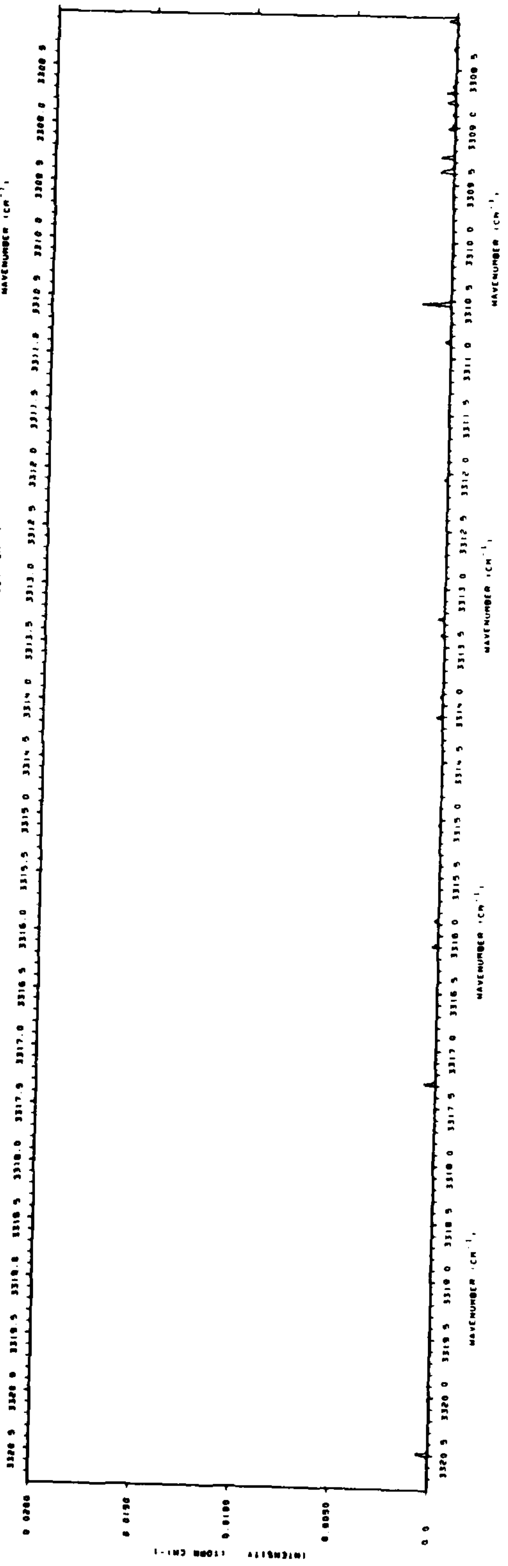


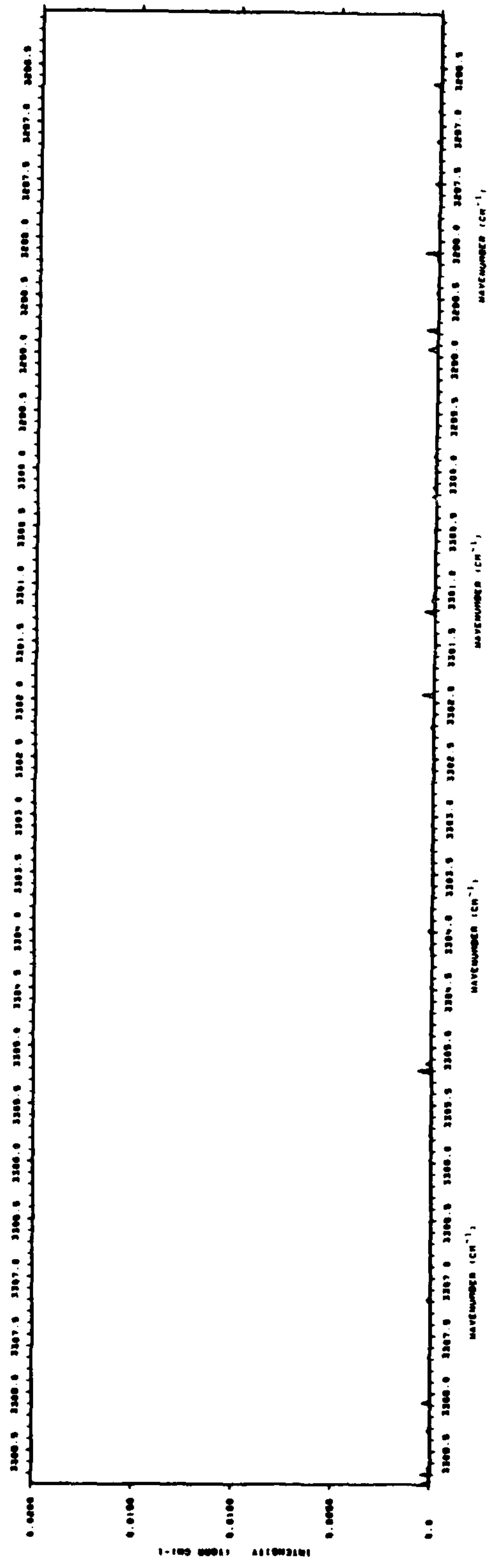


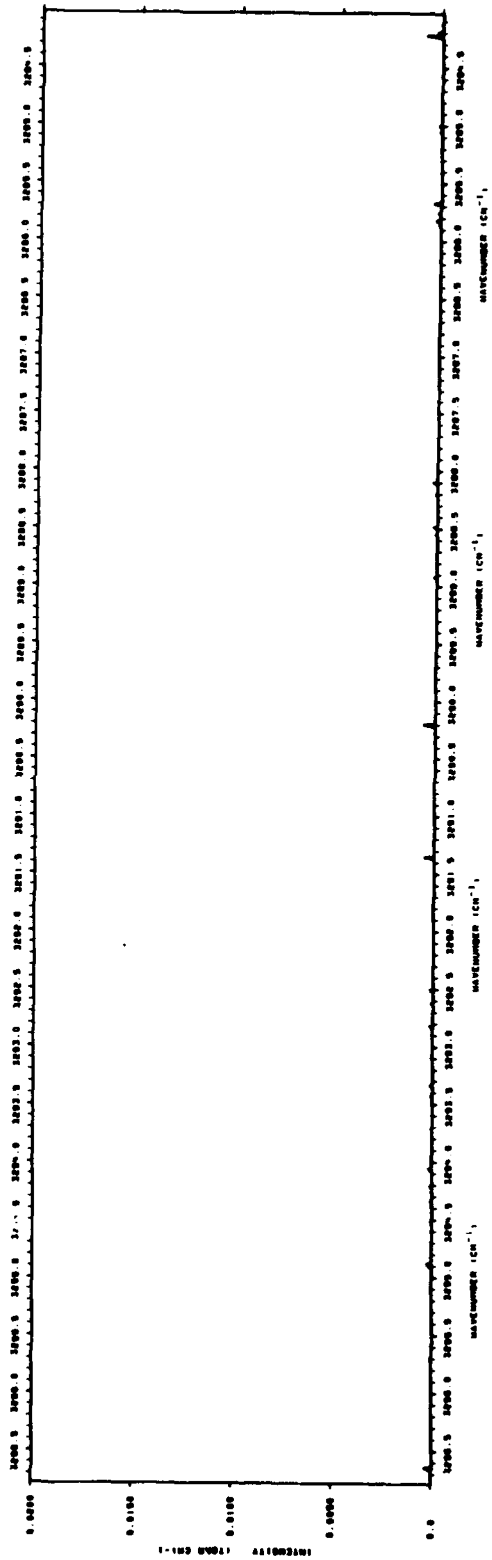


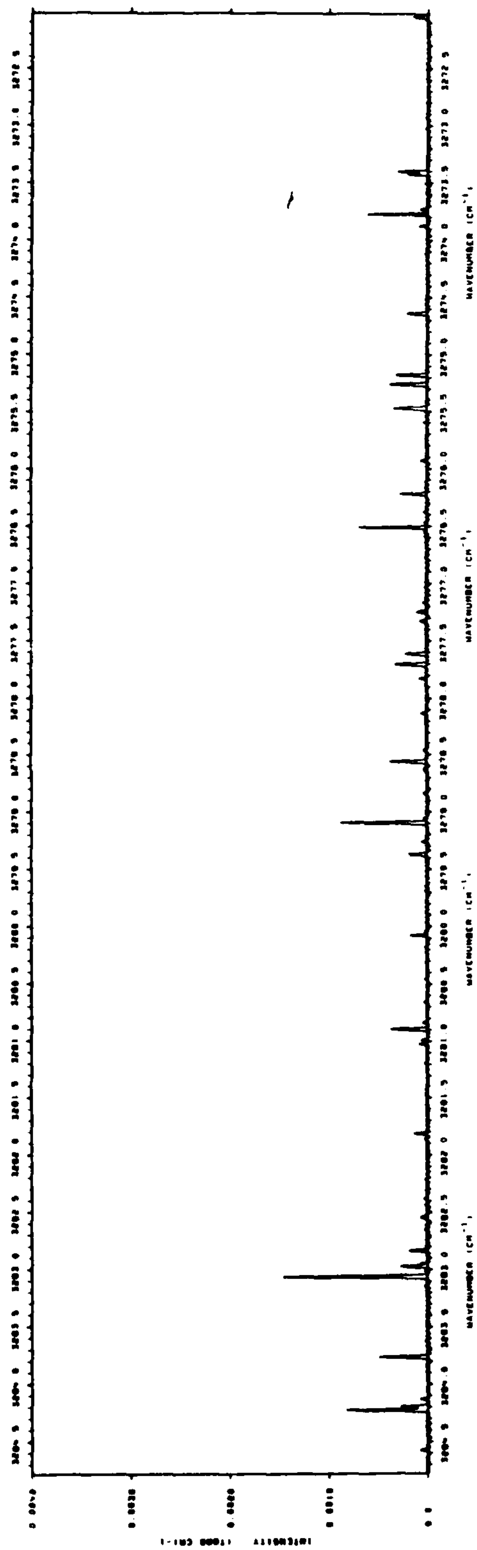


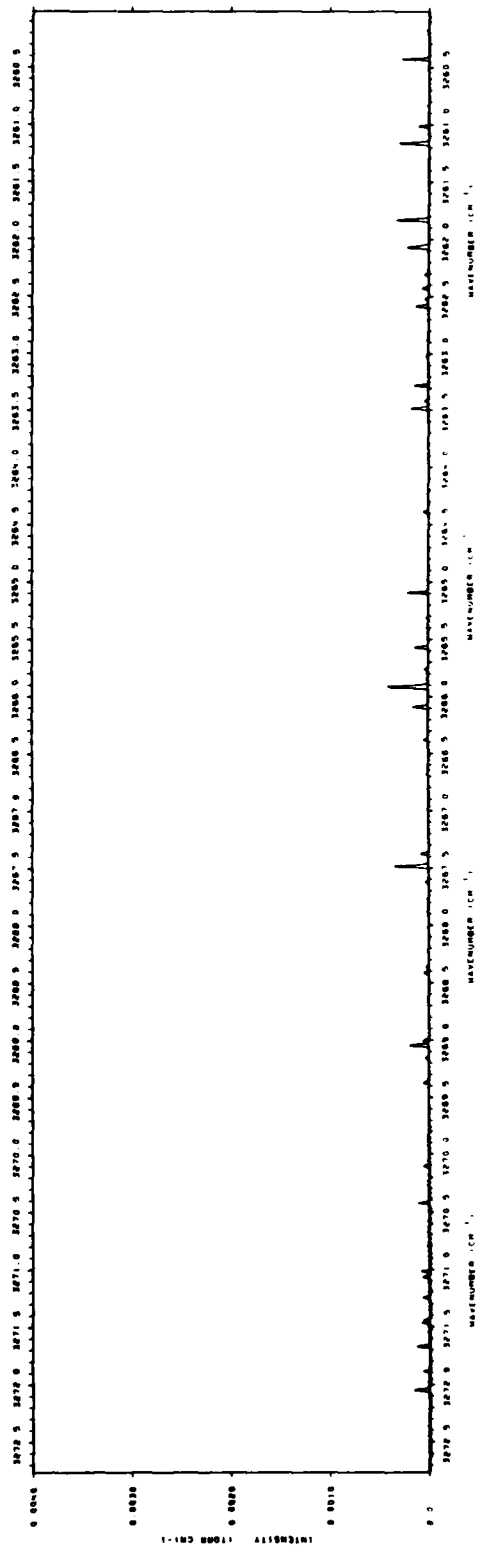


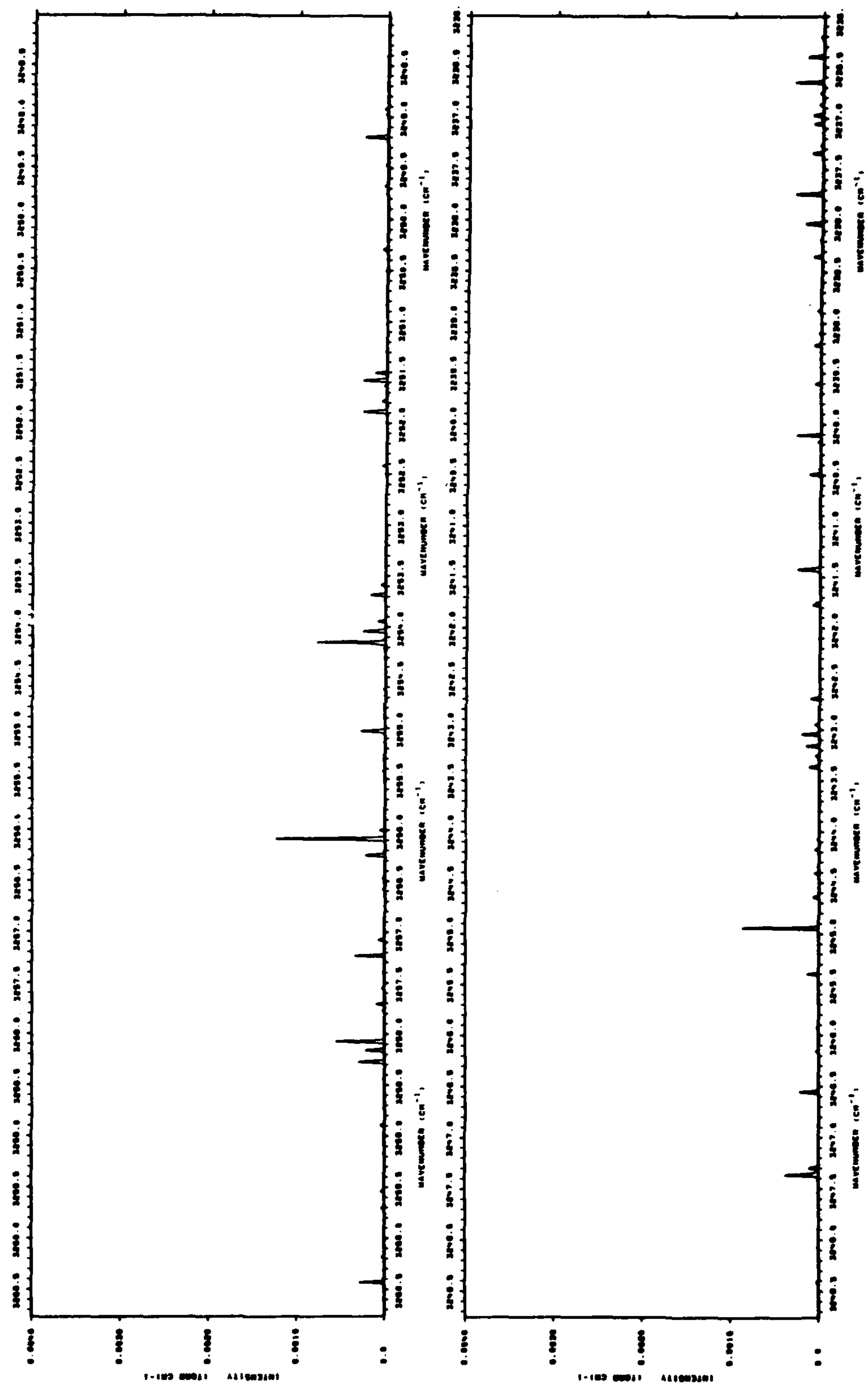


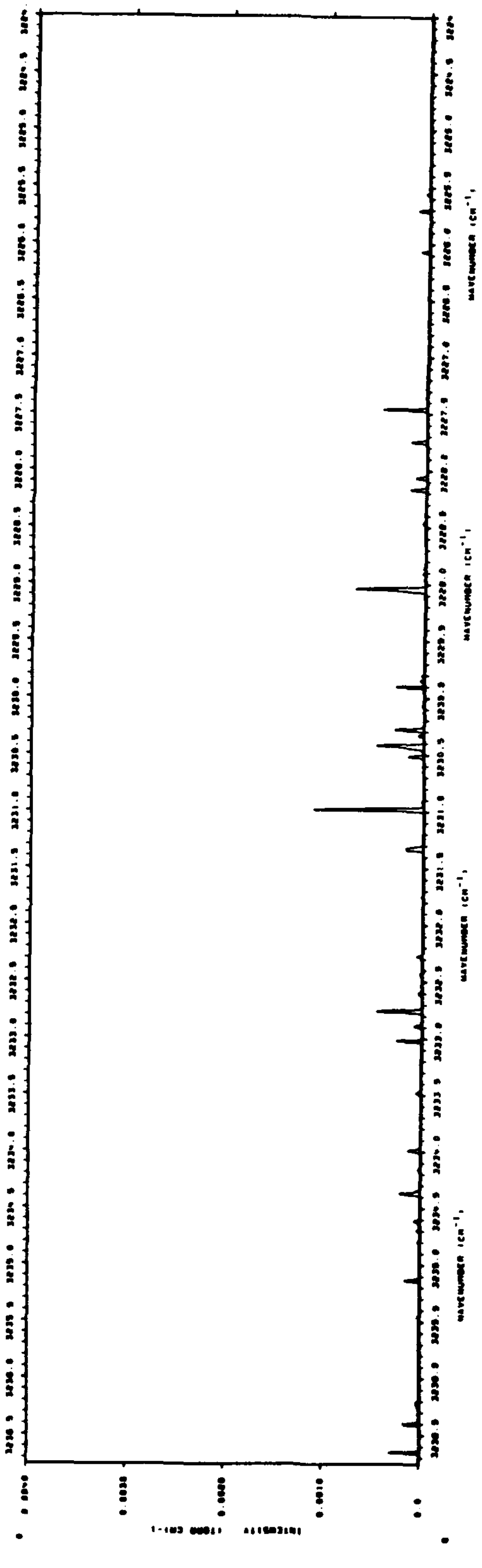


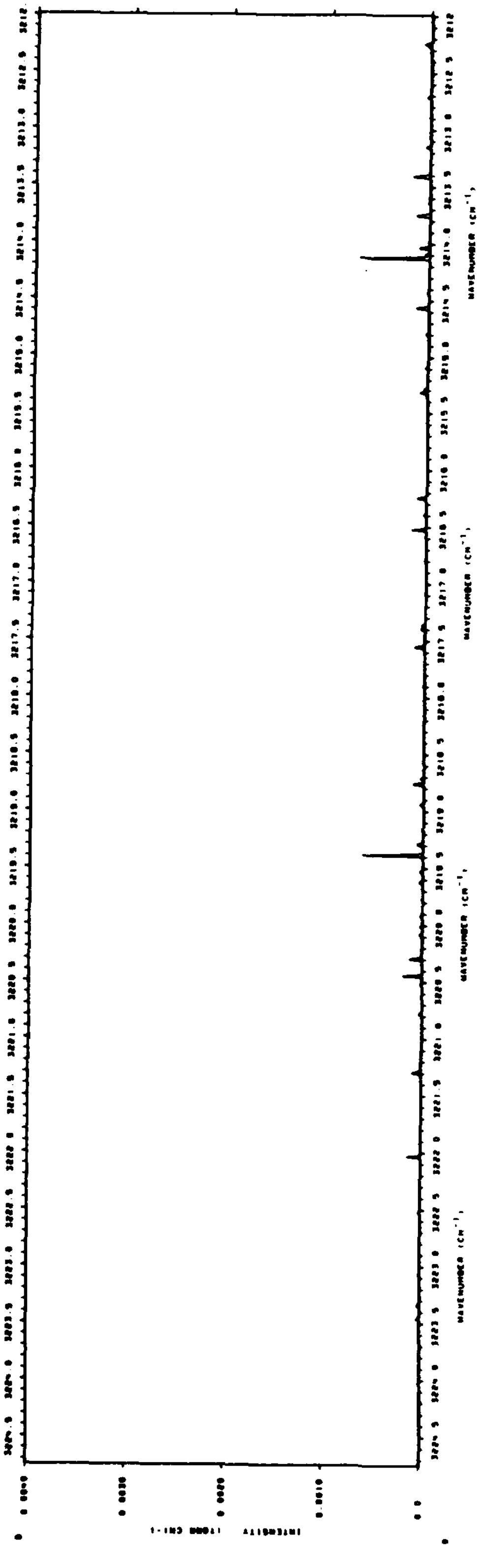


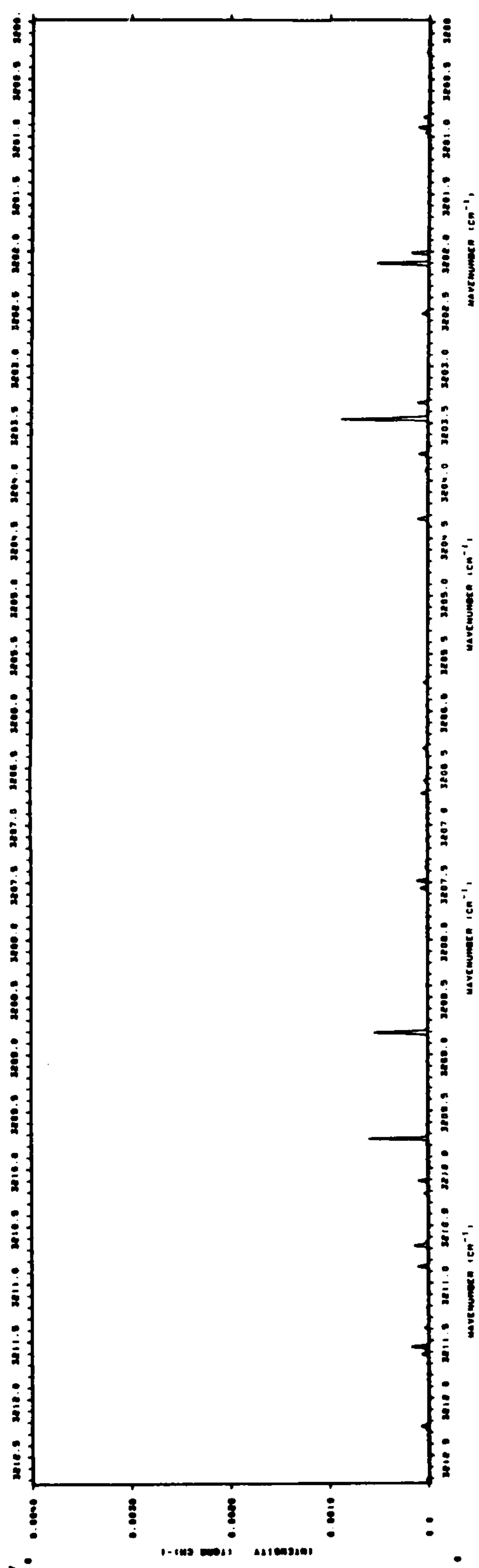


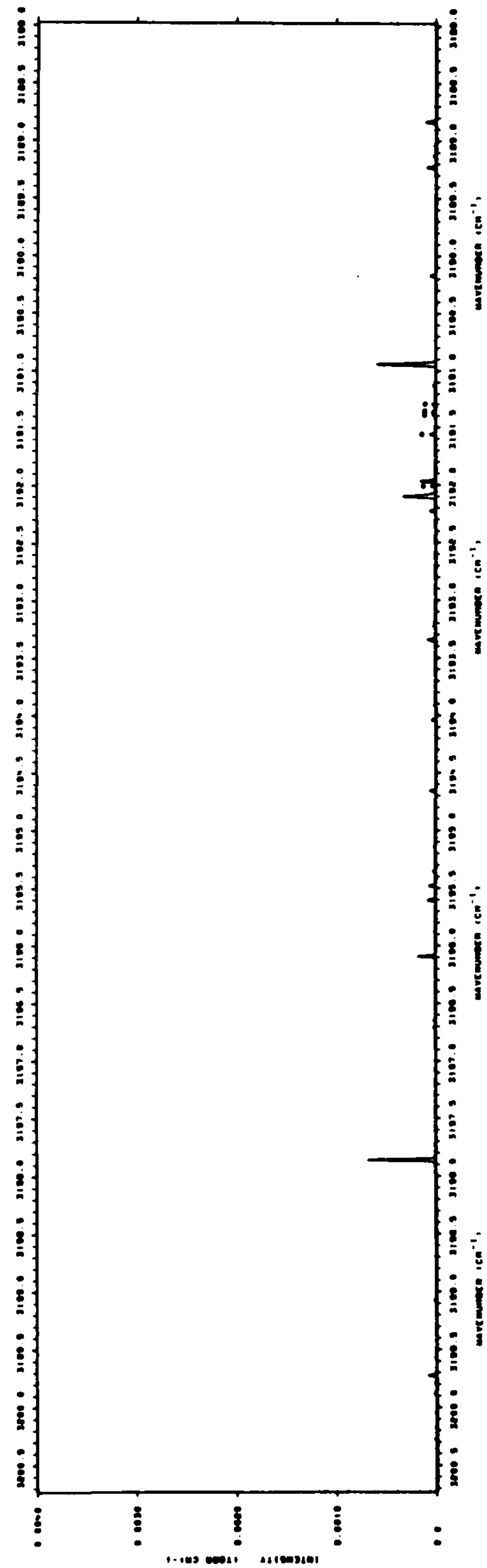


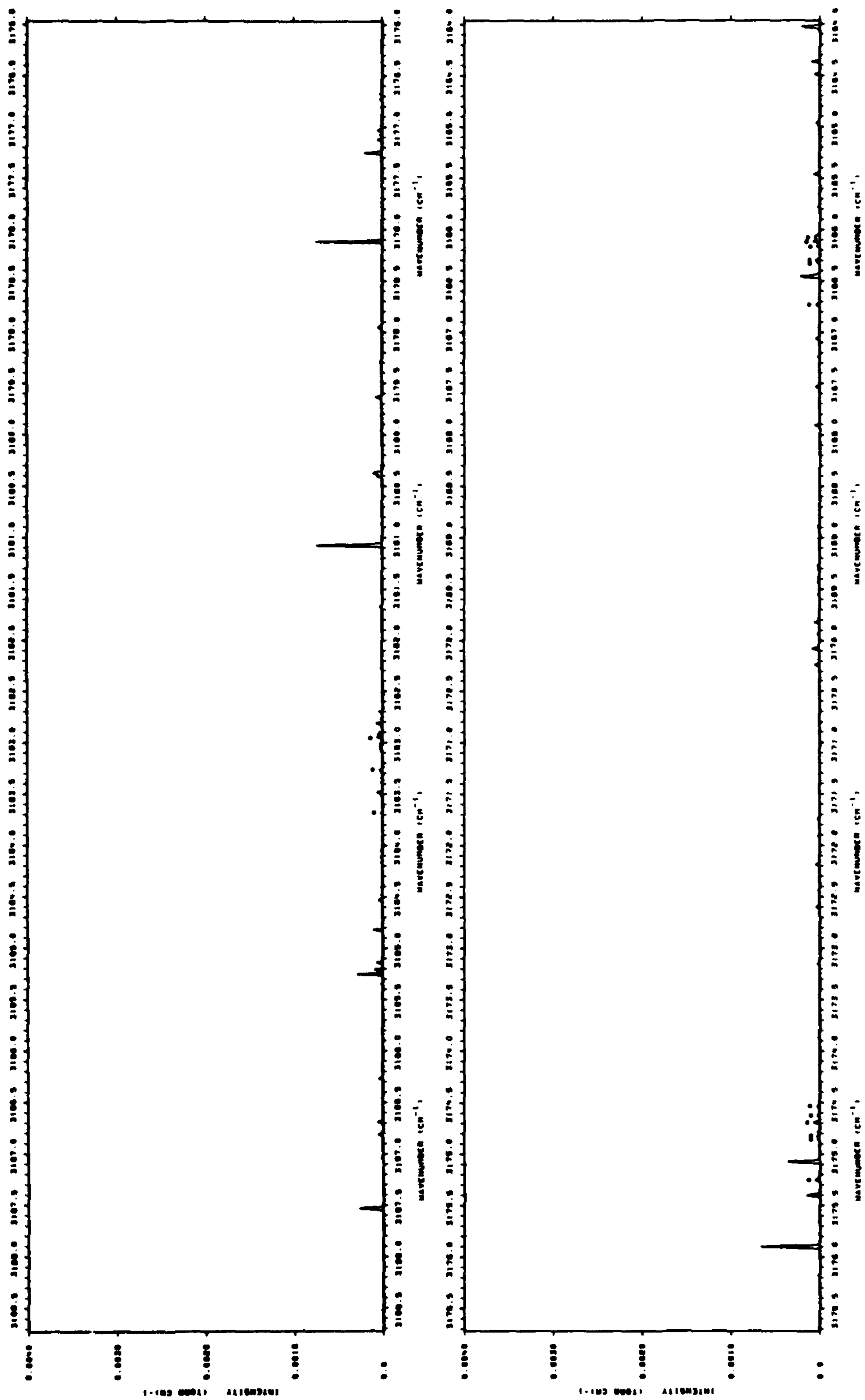


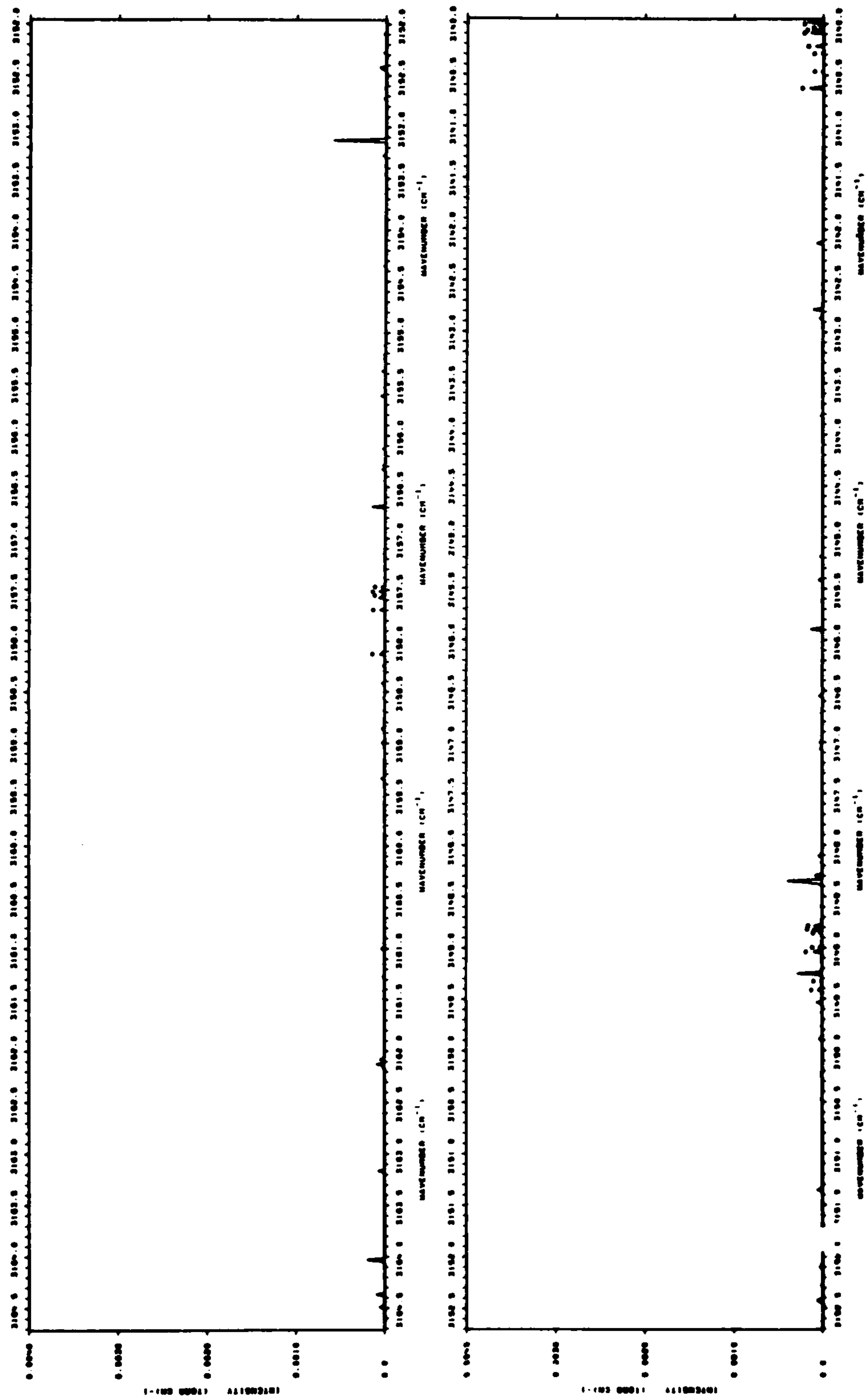


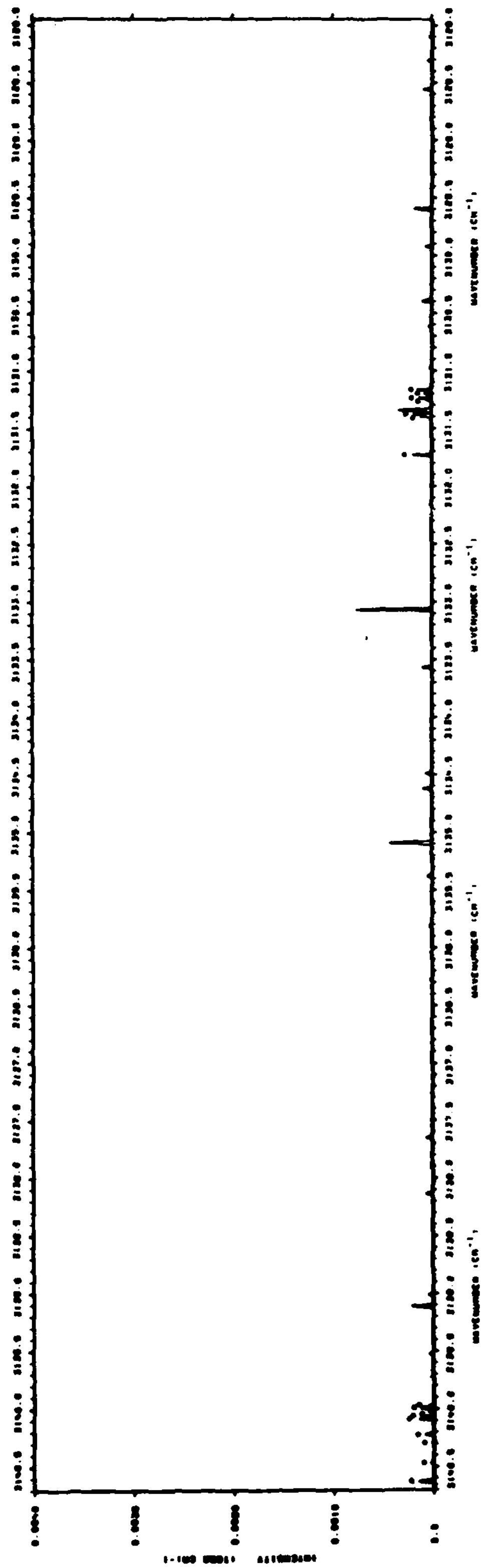


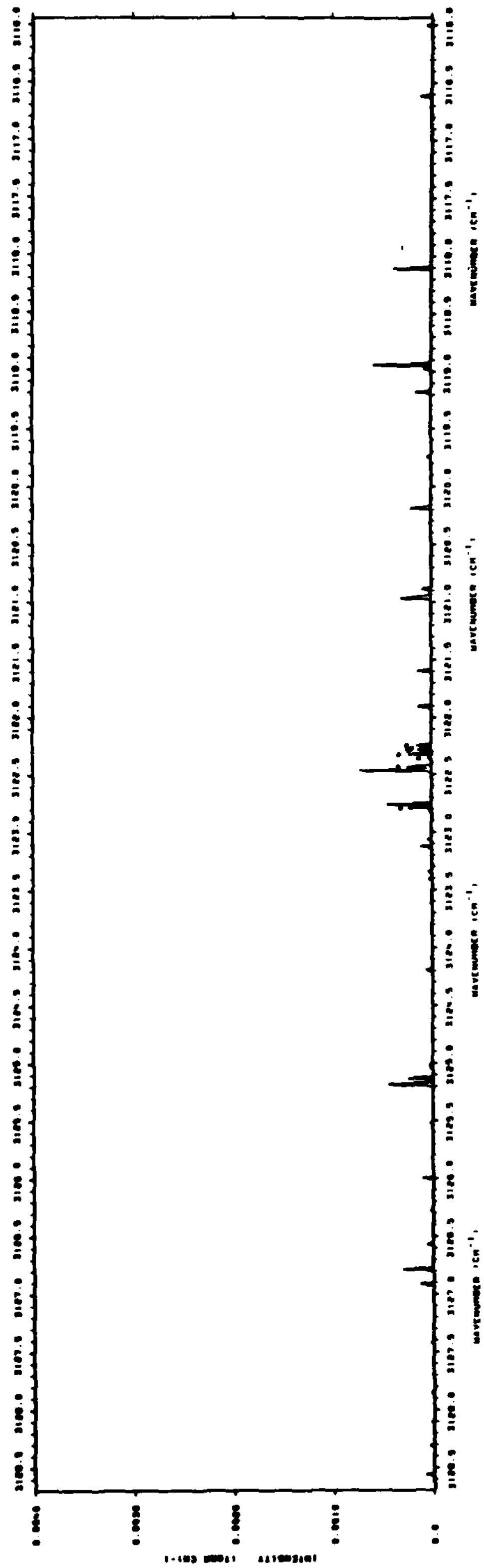


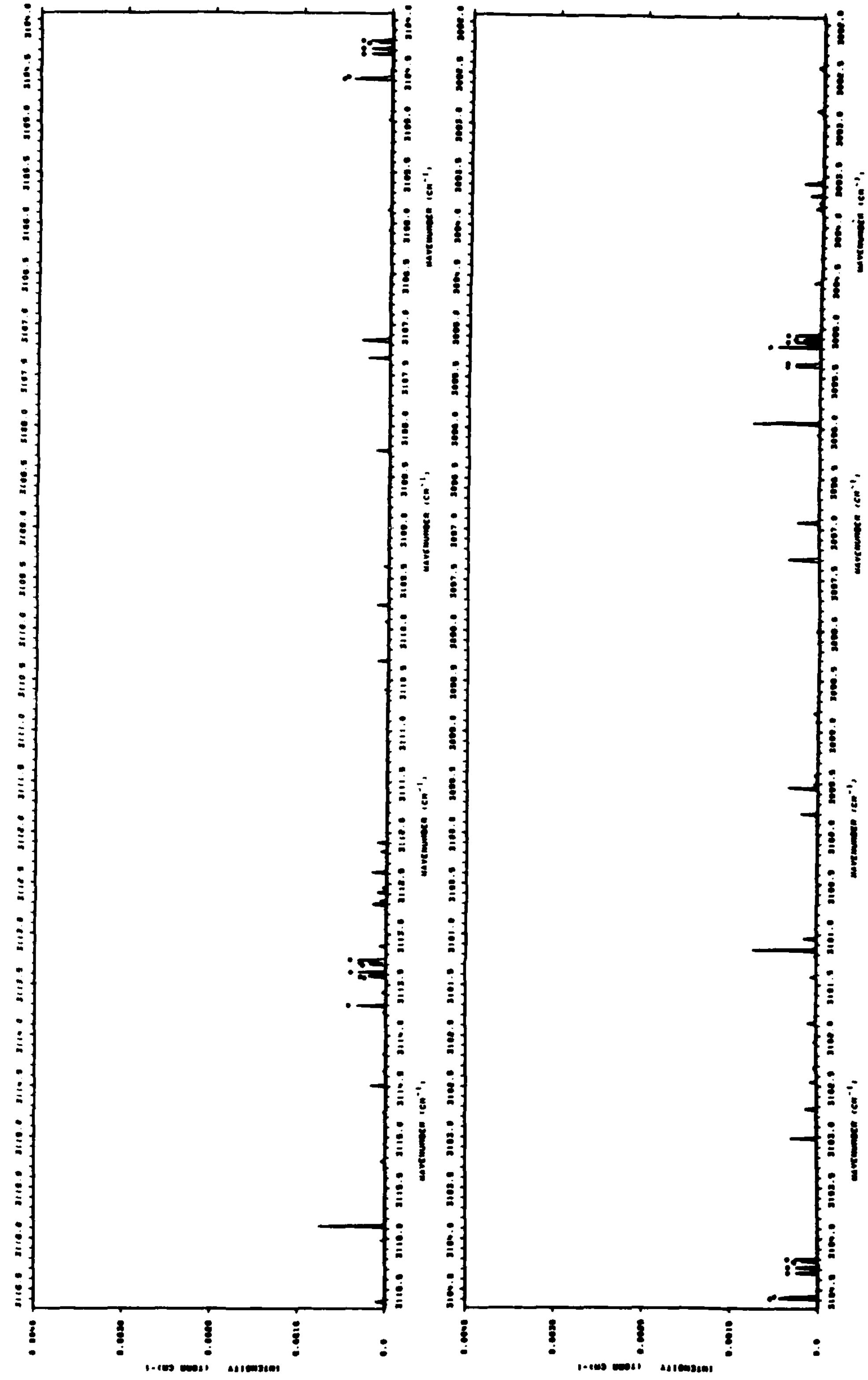


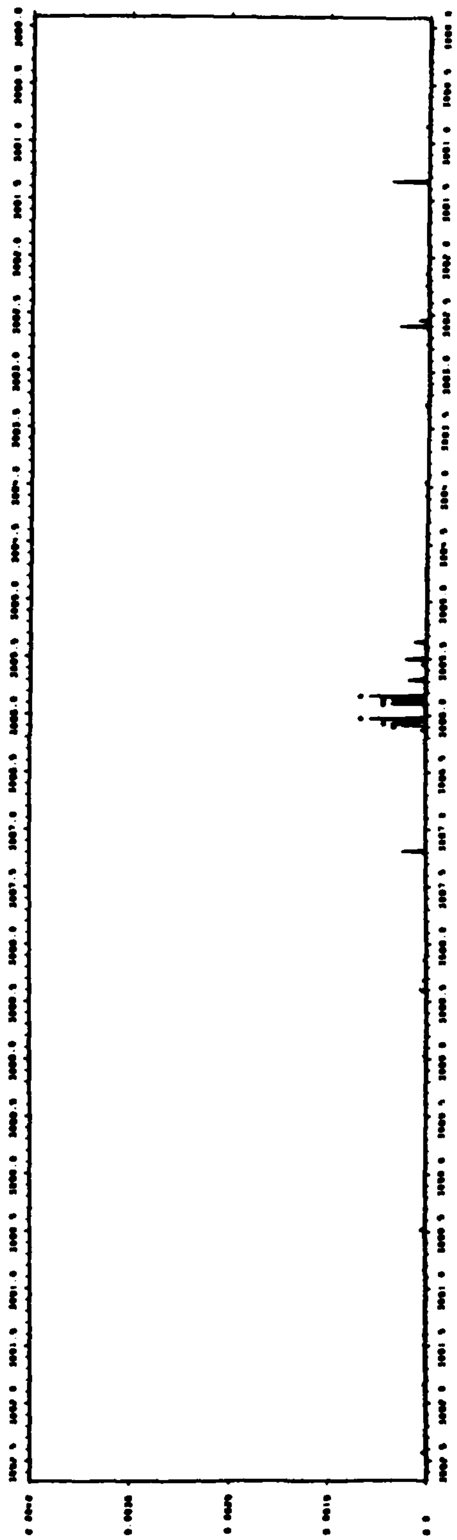


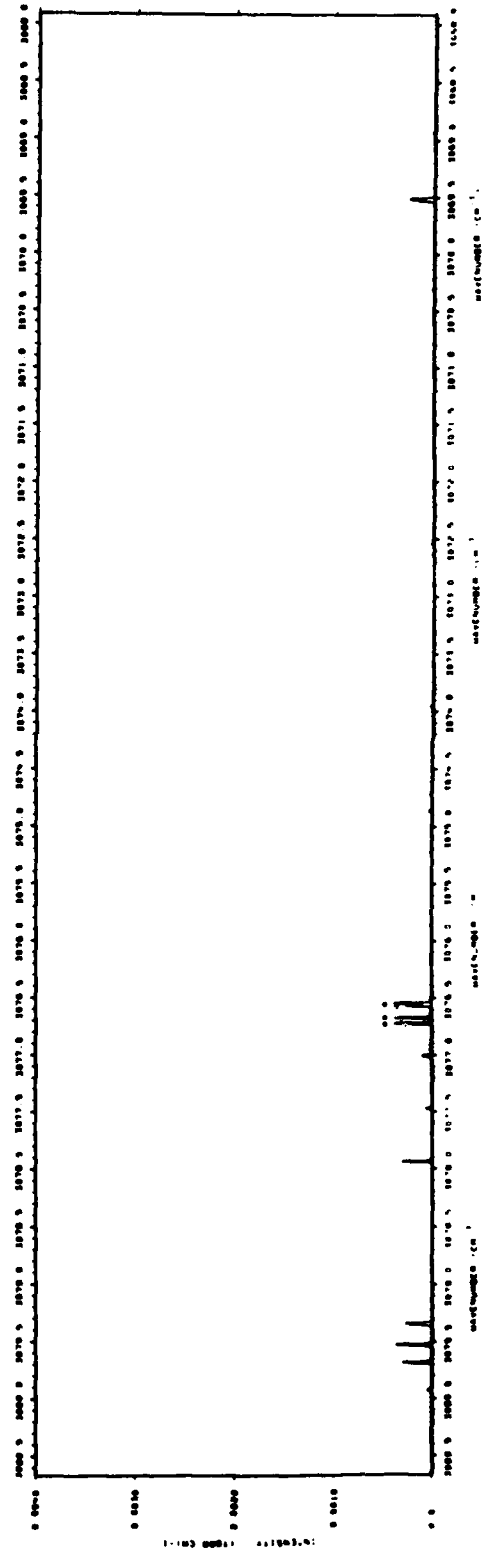


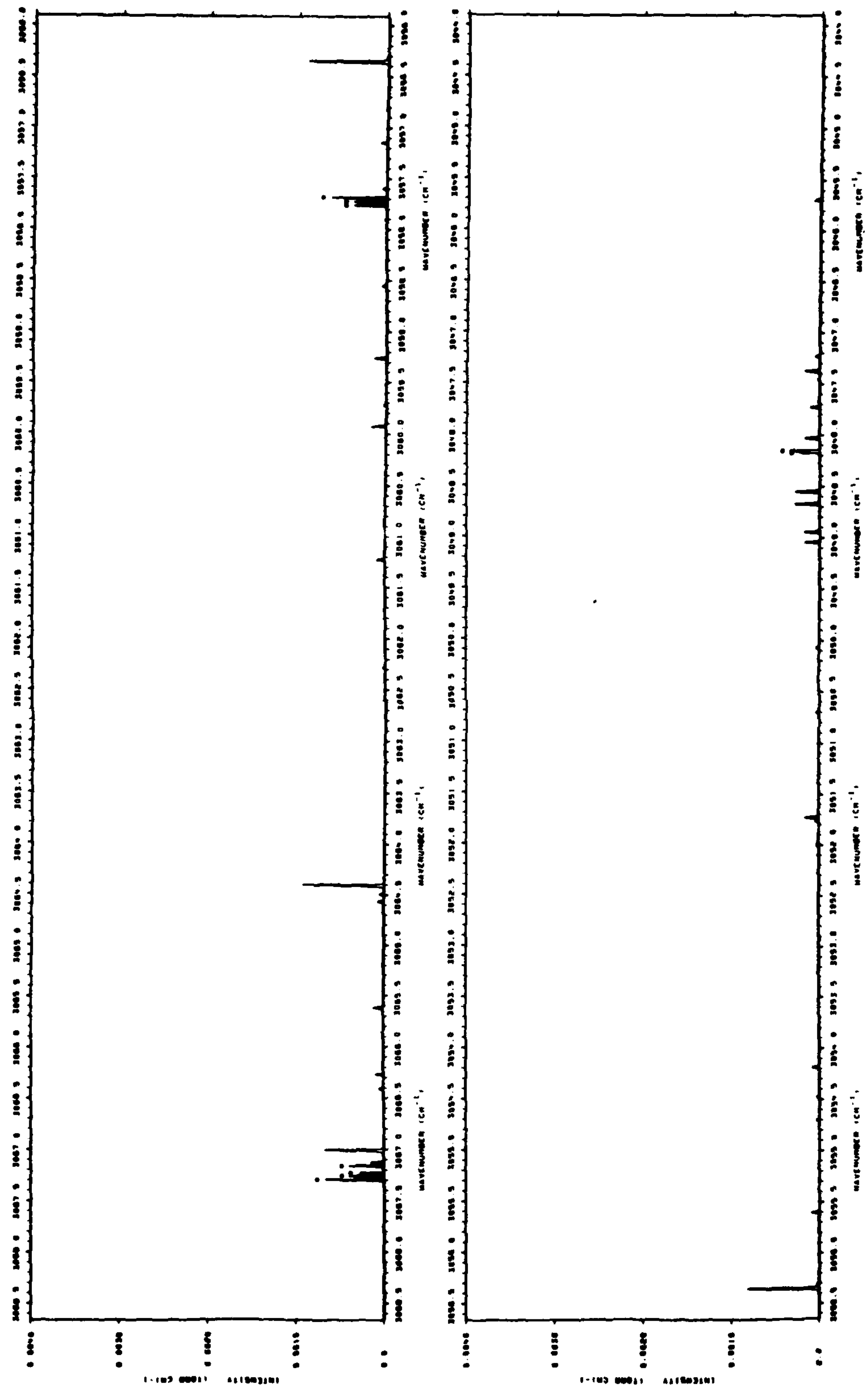


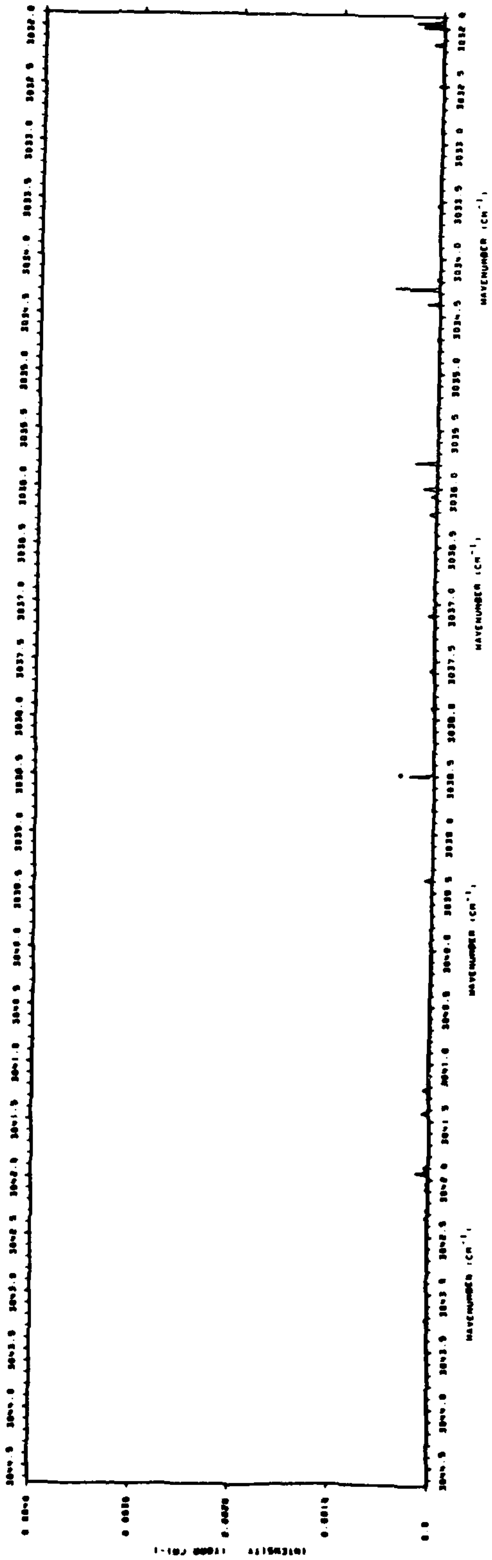


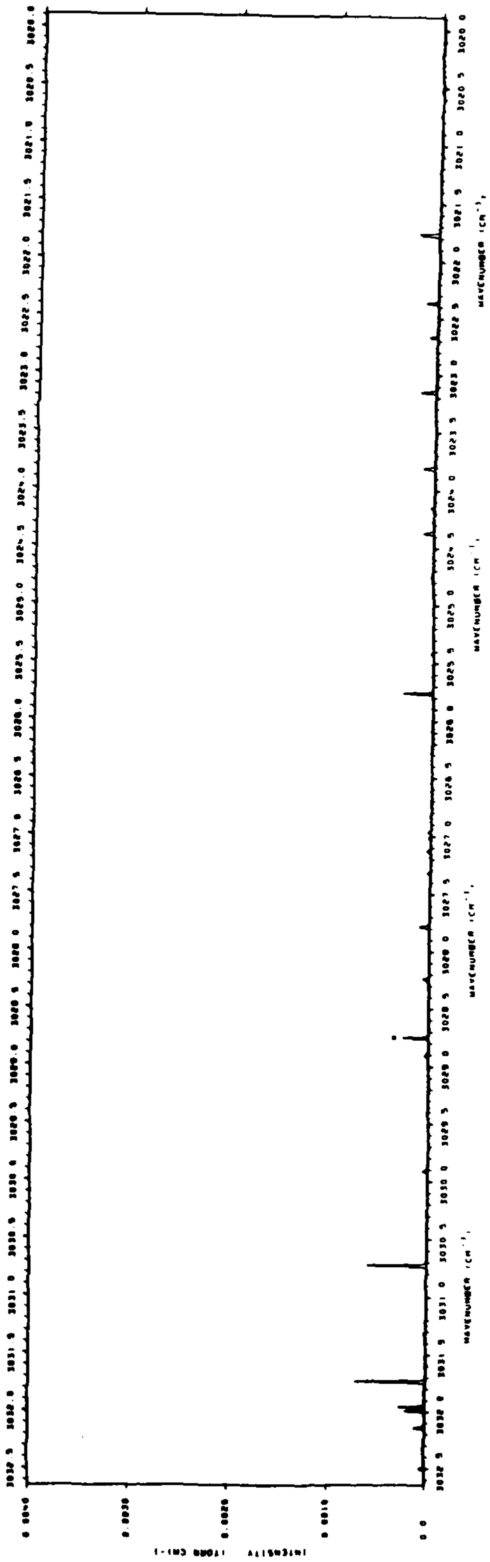


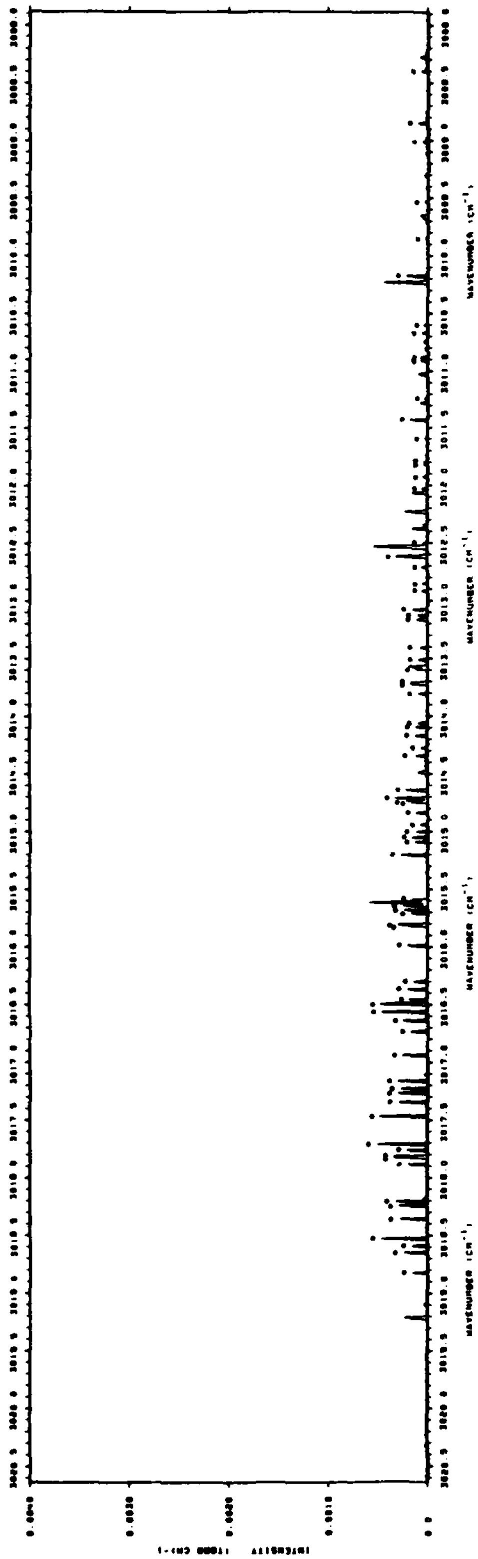


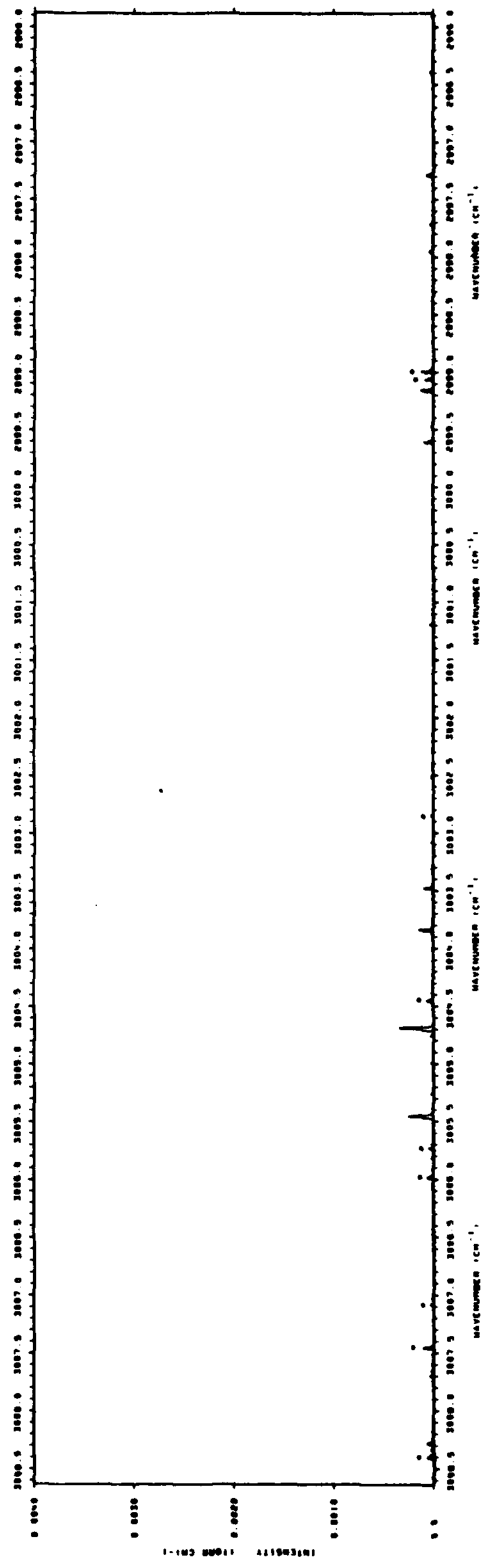


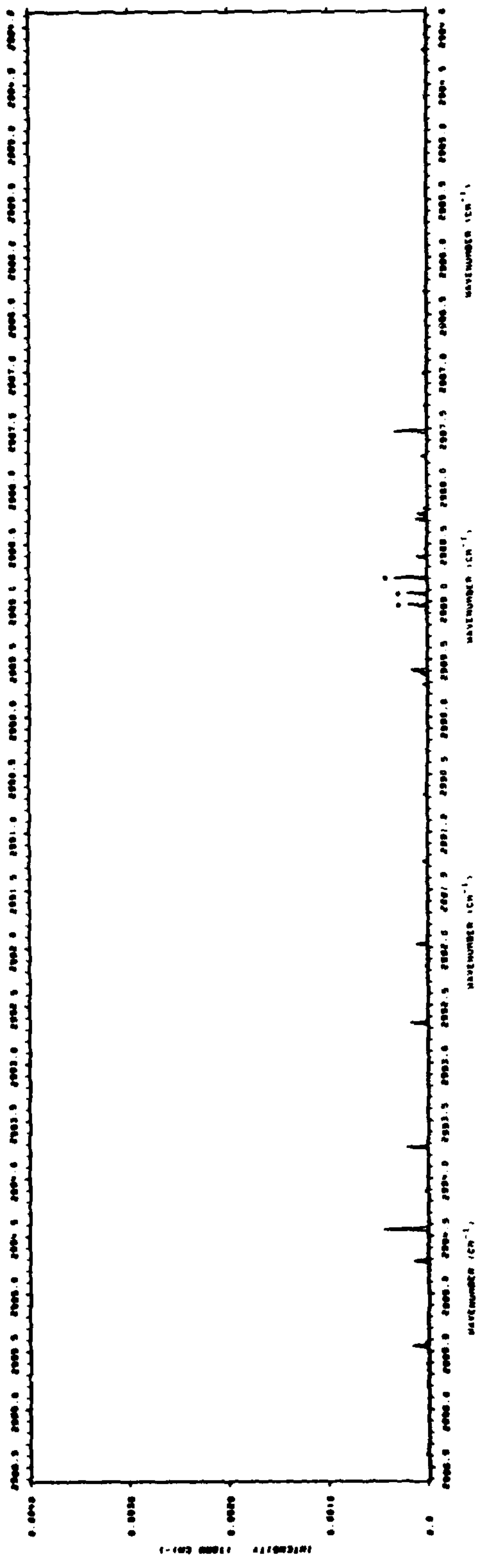


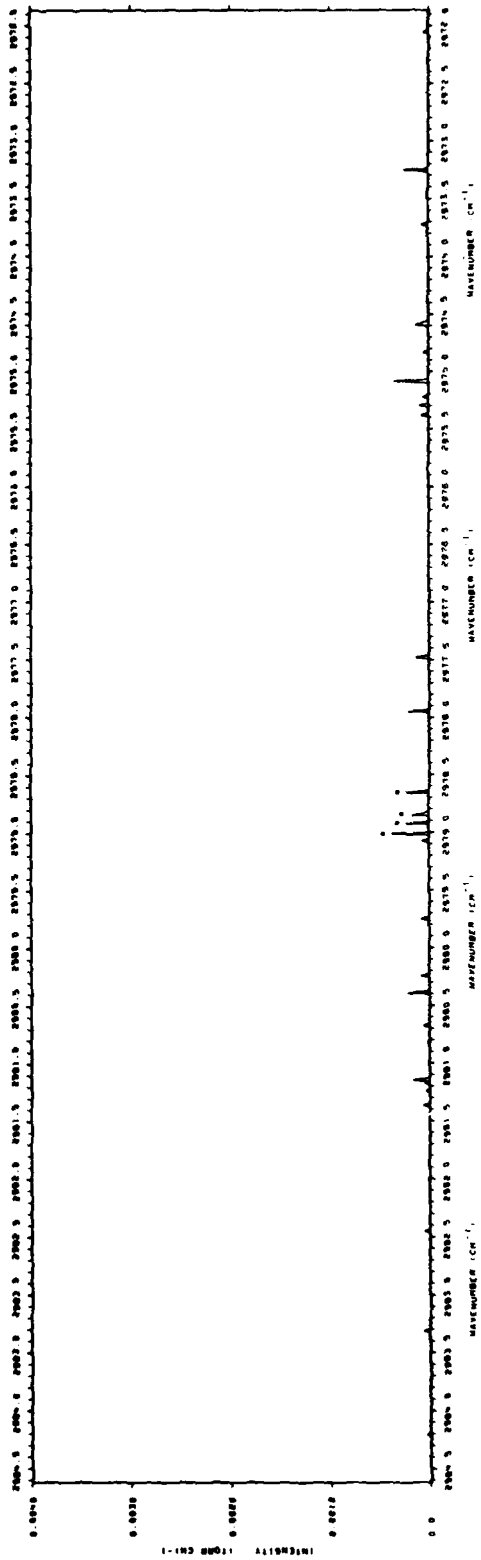


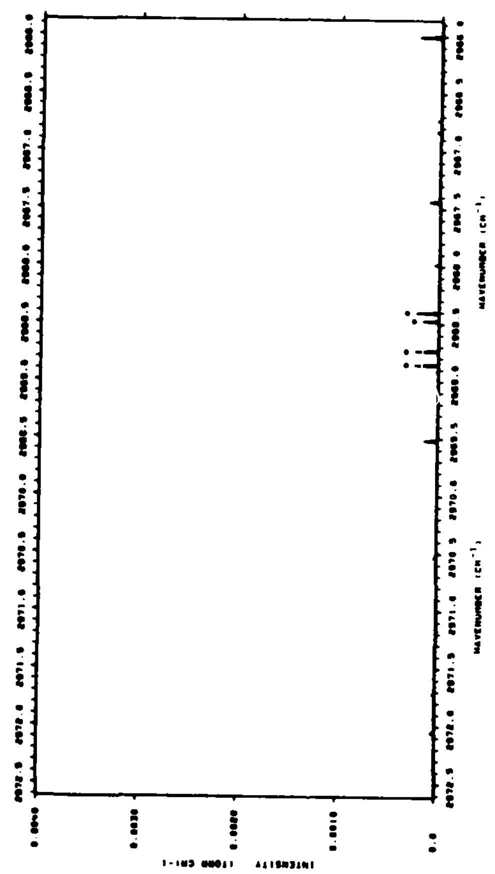












Appendix II.

Listing of Wavenumbers and Intensities of Hot H_2O

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
4004.7052	28	C	0.086	3969.0014			0.045	3939.1121	5	C	0.076
4003.5882	-7	C	0.374	3967.5617	-5	C	0.010	3938.9927			0.010
4002.9667	-11	C	0.257	3967.5000		H?	0.015	3938.4592	10	C	0.007
4002.8608	4	C	0.262	3967.3978	-3	H	0.053	3938.2897	-13	C	0.443
4002.7678	27	C	0.083	3966.7720	46	H	0.045	3938.1096	-2	C	0.118
4001.2814	0	C	0.033	3965.6208	22	H	0.006	3938.0793			0.041
3999.7478	-6	H	0.056	3964.8009	5	C	0.316	3938.0564	-1	C	0.034
3998.8898	18	C	0.059	3964.5295	-8	H	0.009	3935.8594	-48	H	0.005
3998.8323	1	C	0.083	3963.8422	-2	C	0.162	3935.1305	2	C	0.021
3998.7660	-49	H	0.021	3963.0610	-70	H	0.007	3934.4048	-26	H	0.019
3995.9756	-17	H	0.019	3962.1873	1	C	0.267	3934.2628	-61	H	0.033
3995.0275	3	C	0.368	3962.0392	-14	C	1.116	3934.1008	0	C	0.581
3994.8423	27	H	0.114	3961.7115	-16	C	0.800	3932.5820	8	C	1.991
3994.5491		H?	0.007	3961.6565			0.046	3932.5460	1	C	0.770
3994.1114	8	H	0.037	3961.3056	0	H	0.039	3932.1352	-5	C	1.757
3993.9988	-29	H	0.027	3961.1237			0.009	3932.0808	-3	C	0.094
3992.6686	4	C	0.369	3960.6577	-27	A	0.041	3931.3697			0.084
3992.4198	-2	H	0.015	3959.7235	-3	C	0.256	3930.5667	4	C	0.887
3991.1766	-5	H	0.039	3959.5027	-2	C	0.109	3929.7994	-40	H	0.010
3990.7125	-13	C	0.656	3959.1419	-9	H	0.032	3929.3609	-4	C	0.341
3990.4449	34	H	0.021	3959.0199	-10	H	0.096	3929.1287			0.098
3990.2723	-2	C	0.397	3958.3345			0.009	3928.2372	18	C	0.031
3990.2147	-8	C	0.152	3958.2200	-1	C	0.147	3928.2009	-1	C	0.083
3989.8257	-4	C	0.071	3958.1781	13	C	0.013	3928.0871	-16	C	0.009
3989.5693	8	C	0.122	3957.5340			0.011	3928.0302	4	C	0.252
3989.4538	-8	C	0.453	3956.8824	-1	C	0.413	3927.3339	-18	H	0.034
3986.9878	64	H	0.010	3956.2520	3	H	0.029	3926.1240			0.115
3986.5262	112	H	0.009	3956.0588	-22	H	0.059	3926.0683			0.034
3986.4449	11	H	0.034	3955.5691	48	H	0.056	3926.0289	30	C?	0.184
3986.0058	2	C	0.030	3955.2420	4	C	0.165	3925.1765	4	C	1.017
3985.0767			0.012	3954.4571			0.024	3925.1340	-5	C	0.719
3985.0206	3	C	0.076	3954.4165	-39	H	0.069	3924.3735	4	C	0.508
3983.7631			0.011	3954.1571	-21	H	0.030	3924.0608			0.010
3983.4857	-13	H	0.029	3953.7638			0.028	3923.7944	1	C	0.319
3982.8710	10	C	0.015	3953.7062			0.077	3923.4675	-6	C	0.364
3982.7515	2	H	0.037	3953.0971	-5	C	0.133	3923.1632			0.015
3982.2694	-4	C	0.033	3952.3441	-2	C	0.045	3923.0058			0.085
3982.0636	2	C	0.352	3950.8082	-24	H	0.010	3922.9387			0.020
3981.1274	-19	H	0.043	3950.6543			0.005	3922.8331	-21	H	0.060
3980.8347	1	C	0.180	3950.5736	0	C	0.042	3921.4560			0.015
3979.9886	13	H	0.070	3950.1419	5	C	0.202	3920.0884	-7	S	2.475
3979.7704	4	C	0.238	3949.9845	1	C	1.490	3918.0583			0.008
3979.5959	-3	H	0.023	3949.5717	-5	C	0.068	3917.3633	1	C	0.922
3979.3051	16	H	0.012	3948.1771	-2	C	1.180	3917.2847	-16	S	2.428
3976.5728	-7	C	0.079	3947.4648	-50	C?	1.471	3917.2084	-6	C	0.554
3976.2645	9	C	0.772	3947.1746	0	C	0.383	3916.7863	2	C	0.153
3976.0067	0	C	0.536	3946.6099	-6	H	0.070	3916.6056	-1	C	0.014
3975.7780	-17	C	0.203	3944.3685	1	C	0.690	3916.3961	-4	C	0.187
3975.1389	-3	C	0.523	3944.0457	4	H	0.019	3916.3279	-15	C	0.839
3974.7526	-2	C	0.155	3943.0088	8	C	0.015	3915.6687			0.040
3973.9168	0	C	0.061	3942.8860	-12	C	1.098	3915.2553	-7	H	0.015
3973.8062	109	H	0.068	3942.7612	75	H	0.015	3915.1434			0.017
3973.5404	-4	H	0.026	3942.6524	-8	C	1.951	3914.0371	-2	C	0.047
3972.6567	11	C	0.051	3941.6786	0	H	0.075	3913.8538	13	H	0.027
3972.2446	-12	C	0.050	3941.5294	-21	H	0.014	3913.5736	11	H	0.042
3972.1239	-1	C	0.331	3941.2793	37	H	0.032	3913.3166			0.014
3970.6805	0	C	0.156	3940.5899	9	C	0.149	3913.0283	8	C	0.015
3969.9932	-4	H	0.014	3940.4023			0.094	3912.8357			0.004
3969.3329	6	H	0.016	3939.9777	23	H	0.024	3912.7069	5	C	0.050
3969.1385	-3	C	0.799	3939.3985	8	H	0.034	3912.3379	-7	H	0.115

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3911.9526			0.006	3884.8753	-3	C	0.009	3859.0350	-14	C	0.020
3911.7625			0.019	3884.7896	3	H	0.102	3858.1770	0	C	0.038
3911.4267			0.138	3884.0048	-5	C	0.276	3857.4741			0.068
3911.3442			0.044	3883.2662	-9	C	0.828	3857.4242	-13	C	0.433
3910.7732			0.014	3882.9371	12	C	0.017	3857.1639	-9	C	1.296
3910.5387	-16	C	0.006	3882.0692			0.023	3856.7856	17	C	0.049
3908.6281	62	H	0.013	3881.8728	-5	C	0.041	3856.7042	-2	C	0.041
3908.5816			0.023	3881.2762	8	C	0.182	3856.6186			0.021
3907.7526	-6	H	0.065	3881.0285	-3	C	1.502	3856.4460	1	C	0.056
3907.4436			0.047	3880.9531			0.053	3856.2440			0.011
3907.2210			0.016	3880.3552	5	C	1.347	3856.0063	13	H	0.019
3906.1985	1	C	0.274	3880.1911	-10	C	1.874	3855.2834	-7	C	0.017
3906.1584	7	C	0.086	3880.1415	13	C	0.121	3854.4410	18	C	1.805
3906.0643	-10	C	1.271	3879.9500	0	C	0.503	3854.0895	-9	S	2.049
3905.5844			0.012	3879.7853	-10	C	0.145	3853.5760	-2	C	1.047
3905.3705	-1	C	0.422	3879.4821	-15	H	0.069	3853.0983			0.009
3905.0059	7	C	0.060	3878.5188	152	H?	0.028	3853.0132			0.019
3904.5838			0.031	3877.6798			0.021	3851.6270	16	C	0.007
3904.2948	-1	C	1.955	3877.4257	4	C	0.059	3851.0729			0.014
3904.1679	-11	S	2.469	3876.5646	-3	C	0.033	3850.3085	23	C	0.209
3902.4406	-3	C	0.063	3876.2840	5	C	0.010	3849.8672	0	C	0.090
3902.3086			0.120	3874.4026	0	S	2.258	3849.6519	0	C	0.033
3902.2498	-5	C	1.278	3873.9451	5	C	0.436	3849.5994	11	C	0.299
3901.8451	-23	S	2.520	3873.8837	21	C	0.161	3849.3974			0.012
3901.6653	-17	C	1.381	3873.7247	1	C	0.580	3849.0597	1	C	0.142
3900.6919	79	H	0.026	3872.7369			0.027	3848.8877			0.069
3900.2054			0.010	3871.7979			0.100	3848.5679	-71	H	0.026
3899.4424	5	S	2.623	3871.4968	-4	C	0.550	3847.3956			0.018
3899.2166	-7	C	1.928	3871.4529	-5	C	0.183	3847.3416			0.028
3898.7604	0	C	0.017	3871.0825	5	C	0.092	3846.3998	6	C	0.054
3898.2341	-4	C	0.209	3870.8210	-5	C	0.013	3845.6481			0.006
3897.9739	-2	C	0.203	3870.1356	61	S	2.495	3845.5731	42	H	0.029
3897.5679	7	C	0.081	3869.9249	16	S	0.078	3845.5412			0.011
3897.2454	-4	H	0.022	3869.1931	-1	S	2.342	3845.3529			0.030
3896.7814	8	C	0.027	3868.6597	77	H	0.012	3844.8476	1	C	0.133
3896.6231	-14	H	0.044	3868.6265	4	C	0.013	3844.3295	7	C	0.053
3896.4849	19	C	0.054	3868.5032			0.041	3843.7507	-7	C	1.928
3896.4205	10	C	0.036	3868.3939			0.020	3843.5049	-4	C	0.378
3896.3386	-8	H	0.164	3868.2319	-3	C	0.036	3841.6957	-2	C	0.091
3895.1459	14	C	0.130	3867.7530			0.025	3841.6475	13	C	0.128
3894.9470			0.018	3867.6805			0.009	3841.0453	1	S	2.305
3894.2874	-4	C	0.217	3866.7610	23	C	0.012	3840.1269	8	C	0.430
3894.0622	-15	C	0.652	3866.1094	-2	C	0.213	3839.9303	2	C	0.854
3893.6674	-16	C	0.013	3865.8549	-22	H	0.069	3839.7438	14	C	0.012
3892.9934			0.019	3865.1595	41	A	0.149	3839.4623	0	C	0.182
3892.8271	-6	C	0.120	3865.1106	22	S	2.924	3839.2865	19	C	0.008
3892.1435			0.015	3864.3102	0	C	0.677	3838.4905			0.005
3892.0015	-14	C	0.273	3863.7729			0.036	3837.4531	13	C	0.020
3891.8002			0.042	3863.7292			0.011	3835.8708	-14	C	0.168
3891.3011	9	S	3.068	3863.5553			0.028	3834.9833	3	S	3.288
3889.6439	-2	C	0.008	3863.3196	-4	C	0.175	3834.6887	-18	C	0.066
3888.7245	-32	H	0.054	3862.4916	0	C	0.077	3834.5085	7	C	0.033
3888.0066			0.022	3862.3473			0.014	3833.6907	-6	C	0.122
3887.0310	-2	H	0.018	3862.1795			0.020	3833.5656			0.017
3886.9234	-1	C	0.007	3861.7874	-7	S	2.750	3833.5055			0.029
3886.0767	-10	C	1.905	3861.5848	-39	C?	0.053	3833.3648	32	H	0.040
3885.8689			1.301	3861.5159	12	C	0.027	3831.9671	4	C	0.203
3885.6506	-15	C	1.531	3860.5028			0.045	3831.6855	-14	S	2.616
3885.3669	3	C	0.143	3859.6091	-16	C	0.005	3830.3667	4	C	0.006
3885.2068			0.012	3859.4078	-9	C	0.035	3830.2179	-7	C	0.006

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3830.0580	12	C	0.006	3799.9333			0.052	3766.0574	11	C	0.019
3828.6945			0.010	3799.0471	-4	C	0.080	3765.7602	-3	S	2.508
3828.5906	-1	C	0.051	3798.9333			0.007	3764.5996	5	C	0.131
3827.9997	-3	C	0.184	3798.8007			0.024	3764.0474	3	H	0.025
3827.5043	1	C	0.078	3797.7878	-7	C	0.632	3763.7003	4	C	0.055
3826.7538	-8	C	1.497	3796.4393	-7	S	2.076	3763.0656			0.021
3825.9432			0.020	3796.0829	-2	C	0.151	3762.4758	8	C	0.092
3825.5522	-5	C	0.145	3795.6432	-5	H	0.019	3762.1707	-6	C	0.024
3824.4240			0.021	3795.5038	7	C	0.022	3761.6760			0.005
3824.2809	-2	C	0.173	3793.8259	9	C	0.020	3760.3640	4	C	0.017
3823.5516			0.014	3792.6357	-3	C	0.013	3760.1238	-13	C	0.020
3823.2740	-4	C	0.212	3790.4316	-2	H	0.016	3759.8449	-1	S	2.373
3823.1267	0	C	0.020	3789.6343	-5	C	0.029	3759.2520			0.013
3822.5062			0.009	3789.2770	-6	C	0.050	3759.0507	1	C	1.029
3821.7661	13	S	2.365	3789.2436	-4	C	0.015	3758.8180	-30	D	0.007
3820.7395	3	S	2.594	3788.8098	-2	B	0.024	3758.6200			0.013
3819.9533			0.064	3787.6631	-31	C	0.091	3758.3984	0	C	0.018
3819.9049	2	C	0.462	3787.4215	2	C	0.015	3758.0686	7	C	0.101
3819.8535			0.021	3787.3490	73	H	0.018	3757.9425	-45	D	0.007
3819.6031			0.022	3787.1276	11	C	0.020	3757.6283	-4	C	0.029
3818.7744	1	C	0.194	3786.9406	6	B	0.062	3756.6167	-8	C	1.766
3816.6831	2	C	0.176	3786.6886	24	H	0.026	3756.1314	14	D	0.006
3816.3411	-3	C	0.121	3786.2245	-1	C	0.292	3755.6724	17	C	0.008
3816.0997	78	S	3.113	3785.6877	2	C	0.025	3755.4041	3	C	0.056
3816.0828			1.387	3785.5098			0.014	3754.6655	-1	C	0.022
3815.6682	0	C	0.005	3785.2677	1	C	0.152	3754.3410			0.003
3815.6469	-3	C	0.066	3784.9318	-6	C	0.070	3754.2278	38	D	0.006
3815.5456	9	C	0.020	3784.5835	-6	C	0.595	3753.9695	85	D	0.006
3814.4368			0.027	3784.4609	2	C	0.051	3753.8194	5	C	0.520
3813.7995			0.017	3783.7317	12	C	0.017	3753.6537	4	C	0.015
3813.4924	-1	C	0.050	3782.1802	9	C	0.129	3753.2409	39	D	0.008
3812.7237			0.011	3781.9457	4	C	0.078	3753.0533	83	D	0.008
3812.6627	16	C	0.055	3781.8006	-8	C	0.009	3752.8325	0	C	0.057
3812.3465			0.006	3781.3992			0.014	3752.5011	0	C	1.377
3811.9883			0.014	3780.2058			0.009	3751.4705	4	C	0.167
3811.2569			0.011	3779.7625	-1	C	0.427	3751.4148	138	D	0.008
3810.8245	10	C	0.010	3779.4935	-3	C	1.708	3751.1985	35	D	0.007
3810.3248	-7	C	0.008	3779.1515	10	C	0.040	3751.1409	49	D	0.007
3808.5944	-71	H	0.036	3778.8069			0.019	3751.1122	28	C	0.050
3808.0765			0.011	3778.2634			0.034	3750.9564	0	C	0.380
3808.0191	13	C	0.005	3778.0508	-18	H	0.026	3750.6144	94	D	0.010
3807.5982			0.007	3777.9501	5	C	0.125	3750.3536	10	C	0.031
3807.4412	-15	C	0.008	3776.4442	-9	C	0.030	3750.1447	27	D	0.020
3807.0160	11	S	3.705	3774.4784	11	H	0.024	3750.0771	-9	D	0.007
3806.2142	10	C	0.026	3774.0540	9	C	0.012	3748.9668	3	C	0.020
3806.1118	-11	C	0.005	3773.9271	2	C	0.114	3748.3912			0.010
3806.0500	1	C	0.047	3772.5094			0.011	3748.2126	21	C	0.013
3805.5900			0.014	3771.7895	-1	C	0.048	3748.0828	48	D	0.030
3804.3880			0.008	3771.5632	-1	C	0.139	3747.9596	26	D	0.013
3803.8327	-2	C	0.028	3770.8240			0.011	3747.4931	-4	C	0.063
3802.9659	-3	C	1.005	3770.4556	-2	C	0.117	3747.4293	-3	C	0.943
3802.6757			0.025	3769.9916	25	A	0.323	3747.1948	48	D	0.024
3801.9427			0.061	3769.8903	5	S	3.210	3747.0088	18	D	0.015
3801.6644			0.065	3768.9416	13	C	0.054	3746.8346	36	D	0.015
3801.4237	41	S	3.325	3768.6908	9	C	0.041	3746.6151			0.004
3801.4249			0.028	3768.0936	12	C	0.052	3746.3230	-3	C	0.196
3800.9598			0.016	3767.4651	7	C	0.045	3746.2824	44	D	0.027
3800.8771			0.008	3766.8269			0.011	3746.1318	-2	C	0.042
3800.8169			0.039	3766.7497	6	C	0.135	3745.9116	16	D	0.015
3800.4418			0.281	3766.5996			0.014	3745.6845	35	D	0.015

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4} CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3745.5526	-9	C	0.007	3731.3497	-4	C	0.189	3715.7806			0.010
3745.4857	0	C	0.107	3730.9896	6	D	0.202	3715.5559	-1	D	0.017
3745.3457	27	D	0.031	3730.7006	-14	D	0.016	3715.1948	-7	H	0.030
3745.0848	-27	S	2.916	3730.6799	-1	C	0.007	3715.1520	-24	D	0.012
3744.7252			0.186	3730.5786	-114	H	0.049	3714.7945	-11	S	2.634
3744.1849	-1	C	0.347	3730.4767	-1	C	0.038	3714.2958	-12	D	0.015
3743.6383	13	D	0.013	3730.0901	0	C	0.243	3713.8824	44	H	0.021
3743.5639	-15	C	0.018	3730.0194	-6	D	0.010	3713.4610	-10	D	0.016
3743.4044	24	D	0.050	3729.7127	7	D	0.214	3713.4121	-5	C	0.020
3743.3137	27	D	0.015	3729.2578	14	C	0.107	3713.2146	-4	D	0.038
3742.9248			0.005	3728.9095	0	C	0.006	3712.9919	-7	C	0.006
3742.4623	3	D	0.019	3728.8651	16	C	0.063	3712.8687	-28	C?	1.289
3742.3970	10	D	0.062	3728.7462	-63	H	0.029	3712.7099	5	C	0.071
3742.0918	18	D	0.020	3728.5564	-16	D	0.010	3712.5823	-17	D	0.015
3741.3657	7	D	0.074	3728.4104	4	D	0.214	3712.4283	7	C	0.204
3741.3063	-6	C	1.361	3727.9397			0.006	3712.3792			0.064
3740.9899			0.007	3727.7976	-24	D	0.009	3711.8762	-3	C	0.187
3740.8472	22	D	0.023	3727.7375	-7	C	0.880	3711.7474	4	D	0.020
3740.8132	-7	C	0.224	3727.0834	4	D	0.214	3711.7280			0.016
3740.7759	13	C	0.010	3726.4780	6	C	0.084	3711.6223	3	D	0.074
3740.3933	-1	C	0.205	3726.4499	6	C	0.076	3711.4891			0.048
3740.3119	9	D	0.079	3725.7307	7	D	0.210	3711.3472			0.015
3740.0305	-15	D	0.020	3725.6863	1	C	0.270	3711.1026	-4	C	0.386
3739.9988	2	C	0.039	3725.4656			0.010	3710.9550			0.101
3739.8842			0.007	3724.9753	5	S	2.019	3710.9175	-1	C	0.416
3739.5784	24	D	0.022	3724.8940	-2	C	0.644	3710.8450	-10	D	0.013
3739.2325	5	D	0.100	3724.3524	-6	D	0.201	3710.7818	2	C	0.671
3739.0950	2	C	0.369	3724.1885	-3	C	0.092	3710.7061	5	C	0.218
3738.9993			0.006	3723.9196			0.005	3710.5260			0.004
3738.8661			0.008	3723.3786	-4	C	0.174	3710.0051	1	D	0.122
3738.7767	-13	D	0.020	3723.2736	-1	C	0.373	3709.7781	1	C	0.062
3738.5046	-17	C	0.017	3722.9490	-10	D	0.178	3709.4023	-4	S	2.141
3738.4014	4	C	1.126	3722.8264	-8	C	1.109	3709.1996	10	C	0.109
3738.2863	23	D	0.016	3722.7545	-11	C	0.141	3709.1515			0.026
3738.1294	14	D	0.113	3722.6914	-1	C	0.073	3709.0802	-8	D	0.014
3738.0756			0.037	3722.3268	-4	C	0.254	3708.8369			0.008
3738.0249	8	C	0.019	3722.2182	-47	C?	1.892	3708.5980	4	C	0.132
3737.4971	-9	D	0.020	3721.8778	0	C	0.614	3708.3622	2	D	0.137
3737.0018	18	D	0.122	3721.5215	5	D	0.268	3708.2584	2	C	0.399
3736.9668	-2	D	0.012	3721.1661	18	C	0.010	3708.2076			0.006
3736.1967	-3	D	0.019	3720.3380	-13	H	0.048	3707.4273	-2	C	0.010
3735.9143	43	B	0.033	3720.2688			0.005	3707.2897	-13	D	0.021
3735.8486	6	D	0.143	3720.1323	6	C	0.204	3707.0021			0.005
3735.6247	-13	D	0.013	3720.0686	6	D	0.126	3706.8420	7	C	0.221
3735.4934	6	C	1.796	3719.8579			0.011	3706.6950	0	D	0.162
3735.4453	-1	C	1.161	3719.7628	4	C	0.144	3706.6193	4	C	0.039
3735.4077	5	C	0.276	3719.4676			0.014	3706.5505	-12	C	0.235
3734.9324	11	S	2.446	3719.2769	-11	D	0.006	3706.4575	-5	D	0.017
3734.6717	7	D	0.152	3718.9636	-4	C	1.471	3706.4161	-11	C	0.019
3734.6454	-2	C	1.724	3718.5892	2	D	0.093	3705.7501	0	C	0.055
3734.2732	-2	C	0.945	3718.4639	-1	D	0.007	3705.7232	75	H	0.064
3734.0613	31	C	0.013	3717.8112	-8	C	0.008	3705.4736	-14	D	0.020
3733.4995	5	D	0.013	3717.7616	-44	H	0.017	3705.4390	7	C	0.141
3733.4689	9	D	0.177	3717.6418	-22	D	0.011	3705.3561	8	C	0.077
3733.0038			0.005	3717.0856	6	D	0.056	3705.0897	10	C	0.085
3732.8712	2	D	0.013	3716.5968	-6	C	0.036	3705.0015	-5	D	0.182
3732.7380	-10	C	0.066	3716.3132	-4	C	0.030	3704.6481	11	D	0.018
3732.2840	0	C	0.552	3716.1601	-2	C	0.342	3703.6326	-4	D	0.019
3732.2421	11	D	0.185	3716.0174	-8	H	0.094	3703.2842	2	D	0.194
3731.4585	5	D	0.016	3715.9826	-4	D	0.012	3702.8139	-1	D	0.017

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3702.5825	-2	C	0.130	3688.2210			0.050	3668.8395			0.205
3701.8057	-1	S	2.230	3687.9846	16	D	0.008	3668.7776	6	S	2.795
3701.7652	-3	C	0.440	3687.3874			0.021	3668.6950			0.082
3701.6063	24	C	0.143	3687.3111	11	D	0.011	3668.4148			0.010
3701.5400	-10	D	0.201	3687.1948			0.014	3668.2130	0	D	0.024
3701.4318	3	C	1.453	3686.7127	0	C	0.918	3668.0698	37	H	0.292
3701.1543			0.031	3686.5494			0.009	3666.7008	2	H	0.054
3700.9567	7	D	0.014	3686.2273			0.005	3666.0836	-6	C	0.146
3700.7303	9	C	0.039	3686.0941	6	H	0.190	3666.0423	3	D	0.019
3700.1543	-6	H	0.248	3685.9140	0	D	0.010	3665.4188	0	C	0.008
3699.8710	-20	D	0.014	3685.2717	17	D	0.007	3665.0962	-18	H	0.186
3699.7726	-12	D	0.159	3685.2430	-23	H	0.032	3664.5439	32	H	0.027
3699.4945	-12	C	0.114	3684.7514	-16	D	0.084	3664.3913	-70	H	0.073
3699.2681	-4	C	0.900	3684.6070			0.056	3664.3069	-48	H	0.023
3699.0768	6	D	0.012	3684.5291	8	C	0.284	3664.0086			0.026
3698.8566			0.131	3684.2435	-8	C	0.520	3663.8510	10	D	0.014
3698.8022			0.048	3683.9903			0.019	3663.8059			0.010
3697.9815	-5	D	0.152	3683.8209	59	B	0.006	3663.7497			0.008
3697.9548	-2	D	0.013	3683.2080	0	D	0.007	3663.3882			0.006
3697.4971	99	H	0.028	3682.8290	-3	H	0.065	3663.0449	4	C	0.008
3697.1915	-2	H	0.096	3682.7659	-11	D	0.077	3662.7847	36	H	0.035
3696.8874	0	C	0.480	3681.7122	0	C	0.035	3662.7034	-7	H	0.010
3696.4621	-9	C	0.284	3681.5482	15	C	0.329	3662.2431	51	H	0.008
3696.3367			0.054	3681.1245	5	D	0.006	3662.1087	-25	H	0.019
3696.2727			0.024	3681.0730			0.006	3661.8892	-16	H	0.117
3696.1638	-12	D	0.155	3681.0135	-60	H	0.016	3661.7760	-3	C	0.017
3696.0106	-4	D	0.010	3680.8015	-73	H	0.046	3661.6378	18	D	0.014
3695.6943			0.034	3680.7553	-17	D	0.065	3661.4958			0.005
3695.2470	20	D	0.015	3680.3738	-6	C	0.118	3660.7003	-5	C	0.009
3695.1335	1	H	0.016	3679.8679			0.021	3659.9349	-2	C	0.193
3694.7934	-4	C	0.046	3679.6096			0.016	3659.4020	20	D	0.012
3694.3528	3	C	0.271	3679.5602	42	D	0.011	3658.7868			0.006
3694.3225	-15	D	0.156	3679.4364	-2	C	1.564	3658.7486	-78	H	0.013
3694.2933	33	B	0.098	3679.2469			0.029	3658.5629			0.031
3694.0413	-7	D	0.010	3678.7218	-22	D	0.056	3658.4466	-7	H	0.068
3693.7690	-13	C	0.127	3678.6287	25	H	0.187	3657.1483	53	D	0.008
3693.6273			0.040	3678.4920			0.008	3656.7337	-12	C	0.020
3693.2941	1	C	0.076	3677.4376	-10	C	0.616	3656.3034	-6	C	4.060
3693.2364			0.011	3676.6661	-7	D	0.044	3655.9670			0.017
3692.7011	11	C	0.109	3675.6054			0.021	3655.7581	0	C	0.173
3692.4922	11	C	0.029	3675.5266			0.095	3654.8694	54	D	0.009
3692.4566	-14	D	0.133	3675.4828			0.030	3654.8000	74	H	0.034
3692.1606	-7	H	0.038	3674.6967	-4	C	0.311	3654.4292			0.012
3692.0476	6	D	0.011	3674.5873	-7	D	0.035	3654.3210	17	C	0.099
3691.6974			0.053	3674.3471	-4	C	0.020	3653.9203			0.021
3691.4597			0.158	3674.2683	-11	C	0.688	3653.8483	-10	H	0.254
3691.3977	-7	C	0.204	3673.6217	12	H	0.018	3653.6449	-16	H	0.085
3691.2964	-2	S	3.155	3673.0908			0.025	3653.1553			0.006
3691.0620	-5	C	0.032	3672.6980			0.014	3652.9117	-9	C	0.143
3690.9094	-1	C	0.082	3672.5942			0.021	3652.7015			0.021
3690.6314	-2	C	0.267	3672.4854	-6	D	0.032	3652.5743	93	D	0.007
3690.5662	-18	D	0.121	3672.2521	-25	H	0.020	3651.9213			0.026
3690.3116	-7	C	0.272	3672.0945	5	H	0.058	3651.6208			0.054
3690.0276	-4	D	0.009	3671.9276			0.059	3651.5474	9	S	0.221
3689.9057	-23	C	0.048	3671.0439			0.010	3651.3657	2	C	2.468
3689.3290	10	D	0.009	3670.8025			0.482	3650.8434			0.180
3689.0728			0.100	3670.5094			0.129	3650.6363	-1	S	2.757
3688.8045	-7	C	0.037	3670.3604	-6	D	0.025	3649.7219			0.009
3688.7627			0.024	3669.9432	-1	C	0.338	3649.2762	-65	S	3.857
3688.6520	-20	D	0.107	3668.8902			0.039	3649.1893			0.040

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3648.8691			0.010	3629.4473	4	S	2.341	3608.7049			0.007
3648.6671	-10	C	0.147	3629.2775	-35	D	0.107	3608.5834			0.005
3648.5276			0.014	3629.1782			0.050	3608.0766	-34	D	0.057
3648.4788			0.022	3628.6979	-3	C	0.281	3608.0434	-13	C	0.058
3647.9910		D	0.010	3628.3508	32	S	2.389	3607.8971	17	H	0.009
3647.5914			0.111	3627.9656	-24	D	0.113	3607.4218	11	C	0.207
3647.5526	-5	S	2.436	3626.8011	-38	H	0.052	3607.2623	-5	C	0.799
3647.1361	-5	S	2.055	3626.6298	-32	D	0.114	3606.9934	-2	C	1.639
3646.9367			0.032	3626.2060	-2	C	0.704	3606.4450	-40	D	0.070
3646.4637	-1	C	0.906	3625.3940	-41	H	0.027	3605.9847	1	H	0.016
3646.1593	83	D	0.015	3625.2727	-23	D	0.118	3605.9084	-16	H	0.014
3645.9310	-3	C	0.092	3625.1802	9	C	0.046	3605.7226	26	D	0.008
3645.2870	-5	C	0.173	3625.1276	2	C	0.066	3605.6798			0.009
3645.2034	54	D	0.015	3624.2258	-50	H	0.027	3605.6272	12	D	0.008
3644.2233	43	D	0.021	3624.1239	-3	C	0.017	3605.3831	3	C	0.011
3644.0932	-13	H	0.061	3623.8925	-25	D	0.108	3605.2549	-3	C	0.059
3643.3290	-4	C	0.053	3623.2030	0	C	0.053	3604.7933	-27	D	0.083
3643.2190	40	D	0.023	3623.1665	9	C	0.084	3604.5977	17	D	0.008
3643.0251	-3	C	0.072	3622.4893	-37	D	0.103	3604.4450	0	D	0.007
3642.6529			0.013	3621.3457			0.018	3603.9275			0.011
3642.5662	2	C	0.426	3621.1810	4	C	0.846	3603.4513	33	D	0.008
3642.2980	0	C	0.010	3621.0665	-25	D	0.093	3603.3418			0.017
3642.1883	13	D	0.028	3619.9159	-5	C	0.082	3603.2412	-8	D	0.010
3641.7780	-4	C	0.310	3619.6176	54	S	2.407	3603.1186	-24	D	0.092
3641.6431	4	C	0.021	3618.1873	3	C	0.176	3603.0248	-10	C	0.219
3641.1339	9	D	0.035	3618.1517	-33	D	0.064	3602.4905	2	C	0.170
3640.3464	0	H	0.038	3618.0066	1	C	0.293	3602.3538	3	C	0.087
3640.0539	-11	D	0.041	3617.6506	-10	S	2.219	3602.2781	21	D	0.008
3639.9344	6	C	0.074	3617.2943	59	H	0.060	3602.0180	0	D	0.009
3638.9526	6	D	0.048	3616.8316	-19	H	0.023	3601.4214	-36	D	0.103
3638.1126			0.020	3616.6615	-35	D	0.048	3601.0781	-19	D	0.013
3638.0822	0	C	0.343	3616.0055			0.018	3601.0265	-3	C	0.424
3637.8245	-5	D	0.056	3615.9361	24	C	0.014	3600.9580	5	C	0.356
3637.8042			0.030	3615.8147	1	C	0.127	3600.7604	11	C	0.039
3636.6732	-18	D	0.063	3615.6443	-6	C	0.023	3600.2051	0	C	0.025
3636.5639			0.020	3615.5777			0.029	3599.9952	-4	C	0.136
3636.3524	12	H	0.018	3615.3294	6	C	0.032	3599.8481			0.037
3636.2317	-25	C	0.130	3615.2363	-2	C	0.286	3599.7412			0.036
3635.9740	-6	H	0.128	3615.1500	-30	D	0.029	3599.7024	-36	D	0.106
3635.6979	-22	H	0.049	3614.7028	5	C	0.394	3599.5202	0	C	0.064
3635.4997	-13	D	0.070	3614.5102	2	C	1.180	3599.3922	2	C	0.092
3635.4174	7	C	0.016	3614.3789	-12	C	0.017	3599.0571	-1	C	0.172
3635.0222			0.048	3614.3013	5	C	0.067	3598.9763	-3	C	0.029
3634.9828	3	C	0.019	3613.7635	-22	H	0.036	3598.9093	-7	C	0.028
3634.3012	-18	D	0.078	3613.6153	-27	D	0.009	3598.6030	-5	C	0.260
3633.8434	-3	C	1.926	3613.0568	-1	C	0.257	3598.1834			0.016
3633.4500	29	H	0.030	3612.9320			0.032	3598.1352	-4	C	0.324
3633.0803	-17	D	0.090	3612.5622	-4	S	2.307	3597.9626	-34	D	0.111
3632.7046	14	H	0.083	3612.0231	-3	C	0.093	3597.9063			0.029
3632.2762	-5	C	0.089	3611.2756	-24	D	0.020	3597.3503	13	D	0.014
3632.1249	33	H	0.016	3611.1946	-14	D	0.005	3597.1777	-15	H	0.014
3631.8347	-33	D	0.095	3610.8106	-4	H	0.225	3597.0758	-29	H	0.109
3630.9729	-101	H	0.021	3610.3597	-35	H	0.076	3596.9020	-10	D	0.009
3630.8309	4	C	0.242	3610.1702	9	C	0.019	3596.2378	-1	C	0.502
3630.7666	3	C	0.135	3609.9731	-13	H	0.027	3596.2010	-40	D	0.113
3630.5677	-33	D	0.104	3609.7887			0.013	3596.0591	1	D	0.009
3630.2093			0.011	3609.6859	-31	D	0.039	3595.5519	-9	C	0.010
3630.1480	-9	C	0.062	3609.3397	6	C	1.653	3595.4818	-11	C	0.095
3629.9044	4	C	0.249	3609.2350	15	S	2.319	3595.3261	-2	C	1.952
3629.6363	-54	S	4.070	3608.9495	45	D	0.009	3594.7439	-1	D	0.014

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR-M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3594.4162	-48	D	0.102	3580.0942	-5	C	0.562	3563.7079	-11	D	0.011
3594.2842	41	H	0.031	3580.0654	0	C	0.197	3563.5891	-10	C	0.337
3594.2167	-13	D	0.012	3579.3462	11	C	0.147	3562.8159		D	0.011
3594.1285	11	H	0.016	3578.6620			0.016	3562.7209	-11	D	0.009
3593.9734	-10	C	0.051	3578.4976			0.016	3562.4036	-13	C	0.018
3593.4056	-14	D	0.010	3578.0149	6	C	0.013	3562.3203	0	C	0.449
3593.1975	-3	C	1.387	3577.9042	-10	H	0.011	3561.9337	-13	D	0.009
3592.6106	-42	D	0.099	3577.3632	-28	D	0.040	3561.2485	8	C	0.048
3592.0449	-11	D	0.013	3577.2125	-6	C	0.155	3561.1638	2	C	0.040
3591.6090	1	C	0.033	3576.8506	-3	C	0.141	3560.9139	-1	D	0.009
3591.4476	-14	D	0.011	3576.7305			0.013	3560.6421		D	0.009
3590.8617	-13	C	0.012	3576.3608	-22	D	0.005	3560.1327	-2	C	1.322
3590.7835	-35	D	0.096	3575.7729	-31	H	0.019	3559.7374	3	C	0.024
3590.6622	2	D	0.007	3575.3545	-25	D	0.033	3559.6699			0.018
3590.6253	-27	H	0.073	3575.0495	-6	C	0.073	3559.1150	0	C	0.073
3590.4308	-6	C	0.224	3574.7986	-18	H	0.127	3559.0827	-3	D	0.009
3590.3057			0.019	3574.4871	0	C	0.153	3558.4437		D	0.007
3590.2368	-16	C	0.056	3573.9220	-20	D	0.008	3558.3816			0.040
3590.1663			0.050	3573.8842	-46	H	0.037	3558.3236	-14	D	0.009
3590.0799	18	H	0.010	3573.6562	0	C	0.035	3557.9983	-4	C	0.029
3590.0318	-12	D	0.007	3573.3239	-11	D	0.027	3557.8526			0.011
3589.8905			0.005	3573.1276	1	C	0.116	3557.5518	-4	C	0.013
3589.7241	-2	C	0.069	3573.0876	-14	D	0.008	3557.2297	-3	D	0.011
3589.5903	-15	C	0.030	3572.9493	-3	C	0.007	3557.1297	-2	C	0.093
3589.2795			0.009	3572.7480	-9	C	0.018	3556.4875	-15	D	0.009
3589.2532	-8	D	C.009	3572.2708	-22	D	0.006	3556.2211		D	0.009
3589.1049	-17	H	0.018	3572.2127	-12	H	0.059	3555.3518		D	0.007
3589.0237			0.030	3571.4173	-7	D	0.008	3555.2096			0.015
3588.9332	-38	D	0.087	3571.2678	-22	D	0.024	3554.9147			0.024
3588.7504	3	S	2.443	3570.5399	-5	C	0.539	3554.8859			0.025
3588.7108	2	C	1.333	3570.3175			0.024	3554.7796	-2	C	0.036
3588.5934	-24	D	0.013	3570.2486	26	H	0.212	3554.7189	-83	H	0.010
3588.5471	-2	C	1.458	3570.1722			0.070	3554.6307	-13	D	0.010
3588.3770			0.149	3569.7238	-12	D	0.011	3554.4460	15	C	0.008
3587.9743	-12	C	0.037	3569.3612			0.007	3554.0635			0.017
3587.8220	-20	D	0.007	3569.1911	1	D	0.021	3553.9473			0.028
3587.7779	-13	C	0.480	3568.9065	5	D	0.009	3553.8804	7	C	0.228
3587.4864	-1	C	0.044	3568.7977	-8	C	0.130	3553.8204			0.008
3587.2539	61	C?	0.010	3568.6781			0.041	3553.7378	-3	C	0.696
3587.1081	-1	C	0.119	3568.2899	1	S	2.662	3553.4397	0	H	0.034
3587.0609	-41	D	0.073	3568.0841	5	C	0.042	3552.8060	-11	C	0.055
3586.9550	-1	C	0.861	3567.9228	4	S	2.477	3552.7547	-3	D	0.010
3586.6036	0	C	0.431	3567.1948	-62	H	0.064	3552.4083	-14	C	0.029
3585.6530			0.068	3567.0898	8	D	0.015	3552.2269	-10	C	0.483
3585.6186			0.016	3566.7519	-9	S	2.326	3552.1081	2	C	0.379
3585.2903			0.018	3566.5332	-5	C	0.516	3551.8579	3	C	0.124
3585.2478	0	C	0.216	3566.3306	0	C	0.390	3551.7328			0.008
3585.1658	-42	D	0.067	3566.2687	-3	D	0.007	3551.5315			0.010
3583.7100	2	C	0.086	3566.0805	0	C	0.847	3550.8552	-18	D	0.006
3583.6631	-4	C	0.153	3566.0061	11	C	0.078	3550.7523	-40	H	0.029
3583.3792	9	C	0.025	3565.6715	-12	C	1.733	3550.4114	-10	C	0.092
3583.2497	-33	D	0.06C	3565.4602	-18	D	0.010	3550.2244			0.040
3582.7169	2	C	0.054	3565.0161	-14	H	0.194	3549.6635			0.060
3582.3692	4	C	0.110	3564.9649	29	D	0.015	3549.6366	-36	H	0.191
3582.1539	6	H	0.010	3564.6891	-9	C	0.220	3548.9362	-18	D	0.007
3581.8870			0.011	3564.5821	61	H	0.079	3548.5196	8	C	0.036
3581.6501	-11	H	0.011	3564.5058	-12	D	0.008	3548.3917	0	C	0.172
3581.3091	-39	D	0.052	3564.0612	5	C	0.056	3548.3589	16	C	0.010
3581.1265	4	C	0.091	3564.0178			0.026	3547.6167			0.006
3581.0410	4	C	0.037	3563.9668	5	C	0.049	3547.1577	-1	C	1.343

WAVENUMBER IN CM-1, DIFFERENCE IN 10-4CM-1, INTENSITY IN (TORR-M)-1

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3546.8979	3	S	2.362	3527.0081	-5	C	0.208	3505.5552	2	C	0.165
3546.7437			0.179	3526.6154			0.025	3504.9767			0.006
3546.1158			0.006	3526.5685			0.020	3504.7497	-5	C	0.136
3545.9929	-1	C	0.036	3526.3927	5	C	0.096	3504.4658	-11	C	0.015
3545.9057	-4	H	0.163	3526.3096	15	H	0.119	3504.3445	17	C	0.013
3545.5505	-12	C	0.597	3525.8422			0.016	3504.1650	-8	C	1.369
3545.5055			0.024	3525.6389	0	C	1.854	3503.8211			0.007
3545.2228	-6	C	1.800	3524.9006			0.009	3503.5809			0.015
3545.0376	-4	C	0.715	3524.8362	4	C	0.373	3503.2764	2	C	0.415
3544.9427			0.018	3524.5685	5	H	0.047	3503.1082			0.035
3544.6352	-13	H	0.058	3524.1021	2	C	1.278	3503.0757			0.133
3544.4831			0.009	3523.9720	-10	C	0.487	3502.8750	0	C	0.940
3544.1629	-2	C	0.113	3523.1415	6	C	1.441	3502.4097	7	C	1.039
3543.7189	0	C	0.016	3522.8215			0.062	3502.2277	-7	C	0.021
3543.6593	-2	C	0.323	3522.7748	-5	C	0.016	3501.8250	-5	C	0.351
3543.5957	-14	C	0.086	3522.7413	5	C	0.195	3501.7274	1	H	0.056
3543.0197	2	C	0.036	3522.5718			0.018	3501.5679	0	C	0.774
3542.8928	11	C	0.087	3522.2266	5	C	0.050	3501.5141			0.009
3542.7308	-3	C	0.055	3521.2904	2	C	0.038	3501.4629	2	C	0.032
3542.6380			0.018	3521.1153	0	C	0.030	3501.4078	68	H	0.018
3541.0471			0.004	3520.9647			0.020	3501.2265	0	C	0.028
3540.9567			0.006	3519.8478	-4	C	0.047	3501.0626	-2	C	0.186
3540.8635			0.011	3519.0332	10	C	0.012	3500.8734	7	C	0.013
3540.7090			0.015	3518.9929	8	C	0.145	3500.6776			0.018
3540.6778	11	C	0.017	3517.6755	-4	H	0.019	3500.3197	2	H	0.140
3540.1737	10	C	0.023	3517.4496	-6	C	0.343	3499.7463	-5	C	0.580
3540.0489			0.016	3517.4270	5	C	0.123	3499.5593	7	H	0.012
3539.6909	25	H	0.006	3517.3205			0.031	3498.6013	-9	C	0.011
3539.4157	3	C	0.131	3517.1873			0.011	3497.9845			0.052
3538.8061			0.029	3516.1238	-38	H	0.012	3496.6227	-21	C	0.251
3538.7830	-3	C	0.021	3514.6230	-14	H	0.029	3496.3821			0.039
3538.7155			0.008	3514.5363			0.012	3496.2792			0.008
3538.3496			0.043	3514.4022			0.040	3495.7847	-5	H	0.008
3537.7292			0.043	3514.3188			0.014	3495.1774	2	C	0.163
3537.1964	0	H	0.091	3514.1652	2	C	0.008	3494.9293			0.021
3537.1664	-45	C?	0.058	3514.0451	-4	C	0.035	3494.2625			0.015
3536.8743	43	B	0.015	3513.8325	1	C	0.020	3494.1607			0.006
3536.5254	-5	C	0.562	3513.5357			0.009	3493.6872			0.020
3536.2665	3	C	1.034	3513.1651	-48	H	0.091	3493.4378	-3	C	0.029
3536.1858	9	C	0.061	3513.0718	6	C	0.037	3492.6682			0.006
3535.3159			0.007	3512.6112	10	C	0.010	3491.9598			0.020
3533.4598			0.030	3512.4635			0.021	3491.8956	2	C	0.093
3532.8364			0.013	3512.3766			0.005	3491.7994			0.021
3531.6770			0.014	3512.0832	-13	C	0.017	3491.7367			0.009
3531.3754	0	C	0.349	3511.5944	2	C	0.098	3491.1015	-2	C	0.108
3531.2490			0.008	3511.4293			0.015	3491.0089	-9	C	0.336
3530.9365			0.008	3511.3874	67	H	0.009	3490.5549	-2	C	0.007
3530.7595	-8	C	0.154	3510.6532	1	C	0.273	3490.0221			0.013
3530.0744	4	C	0.015	3510.5012	12	C	0.017	3489.5737	-8	H	0.109
3529.2212	-7	C	0.186	3509.5594	-5	C	0.405	3489.3535			0.010
3529.0555	-9	C	0.470	3509.4214	-2	C	1.291	3489.0834			0.016
3528.8641			0.184	3509.0461	-53	H	0.026	3488.8438	18	H	0.033
3528.1199	-6	C	0.120	3508.8355	-8	C	0.129	3488.3498	-6	C	0.043
3527.9705	0	C	0.057	3508.6730			0.010	3488.3210	4	C	0.106
3527.8255			0.026	3508.3800			0.021	3488.1268			0.011
3527.6412			0.016	3507.8322	-8	H	0.176	3488.0210	-12	C	0.312
3527.5475			0.051	3506.7028	3	C	0.014	3487.8415	54	H	0.028
3527.4960	5	C	0.650	3506.0790	5	C	0.009	3486.6870			0.036
3527.4132			0.016	3505.8662	9	C	0.041	3486.5913	-41	H	0.148
3527.0300	-16	C	0.316	3505.5977			0.017	3486.4700	0	C	0.025

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3485.7408	0	C	0.624	3462.9843	-15	H	0.079	3443.5096	-74	H	0.076
3485.1574	-76	H	0.010	3462.9381			0.034	3443.2037	2	C	0.043
3485.0304	7	C	0.010	3462.8142	-6	C	0.167	3443.1026	1	C	0.381
3484.1319	3	C	0.314	3462.5904	-9	C	0.094	3442.7793	-31	C	0.011
3484.0118			0.013	3462.5241			0.017	3442.6408			0.008
3483.4514			0.018	3462.2952	22	H	0.035	3442.5035	2	C	0.221
3482.7385			0.015	3461.7786			0.017	3442.1752	-19	C	0.010
3482.4809	-7	C	1.015	3461.6983	-7	C	0.161	3442.0781	12	C	0.044
3482.2463	-7	C	0.338	3461.6473			0.015	3441.8730			0.009
3481.6624	10	C	0.011	3461.5556	-10	C	0.013	3440.5236			0.016
3481.5142			0.033	3461.3431	-12	C	0.039	3440.1697	-19	C	0.006
3481.4430	-39	H	0.108	3460.7731			0.014	3439.8020			0.019
3481.1259	0	H	0.086	3460.7169			0.019	3439.7644	44	B	0.120
3480.8864	5	C	0.234	3460.5943	-3	C	0.739	3438.9859			0.011
3480.7566	-16	C	0.044	3460.4085	-6	C	0.676	3438.9508			0.012
3480.6537	-4	C	0.064	3460.2134			0.011	3438.6897			0.019
3480.5937	-11	C	0.890	3460.0158			0.018	3438.6417	9	C	0.410
3480.4724	63	H	0.098	3459.7269	-2	H	0.114	3438.5837			0.136
3480.3954	1	C	0.761	3458.9314			0.017	3438.4485	16	C	0.392
3480.2191	-14	C	0.022	3458.7607	2	C	0.529	3438.2204	-46	H	0.085
3479.7062			0.023	3458.5949	-6	C	0.185	3438.1898	-5	C	0.014
3479.6437	6	C	0.011	3458.5443	-11	C	0.686	3437.7703	3	B	0.228
3479.3700	-6	C	0.230	3458.1357	-21	H	0.026	3437.7372			0.021
3478.6956			0.038	3457.5027			0.006	3437.4789	26	C	0.263
3478.2936			0.007	3457.3762			0.006	3437.4370			0.087
3476.3469			0.005	3457.2496	-6	H	0.090	3437.4014	4	C	0.009
3475.7886	-28	H	0.018	3456.7533	33	B	0.018	3437.1099	-17	H	0.033
3475.0336	6	C	0.109	3456.2543	0	C	0.442	3436.9386	-123	H	0.009
3474.9224	105	H	0.060	3455.7809	-2	C	0.029	3436.8248			0.011
3474.7385	8	C	0.463	3455.6971			0.013	3436.4483	83	B	0.428
3474.1256	6	H	0.016	3453.6879			0.011	3436.2919	11	C	0.459
3473.3683	-11	C	0.019	3453.1281	-19	B	0.185	3435.9793	-17	C	0.144
3473.3458			0.015	3452.3570	-29	H	0.026	3435.8717	-6	H	0.068
3473.2620	0	H	0.009	3451.9627			0.008	3435.7554			0.018
3473.1532			0.007	3451.2368			0.012	3435.6935			0.011
3471.9469			0.014	3450.8855			0.005	3435.5584	34	H	0.023
3471.7943	-3	C	0.154	3450.1909			0.013	3434.0525			0.015
3471.7049	-8	C	0.015	3449.9395	-2	H	0.052	3432.8306	3	C	0.045
3470.8220			0.016	3449.7807			0.010	3432.1302			0.011
3470.5636	-9	C	0.156	3449.5881			0.012	3431.0996			0.007
3470.3410	0	C	0.049	3449.3773	20	H	0.009	3431.0646	0	C	0.063
3470.2531	6	H	0.010	3449.1309			0.008	3430.8908			0.005
3469.0290	45	H	0.015	3448.9421			0.008	3430.8439	16	C	0.006
3468.8677			0.012	3448.7423			0.011	3430.7144	50	H	0.009
3468.7864			0.015	3448.6989	18	C	0.122	3430.2316			0.009
3468.5581	-4	C	0.010	3448.4008	4	C	0.087	3429.5812			0.011
3467.6757			0.012	3448.3637	28	H	0.024	3428.5963	-40	H	0.013
3467.5731			0.009	3448.2330	-37	H	0.010	3428.0792			0.012
3467.4969	18	C	0.005	3447.9878	8	H	0.016	3427.9172	0	C	0.054
3467.1450	-33	C?	0.051	3447.6145			0.009	3426.8485			0.054
3466.8951	4	C	0.238	3447.2361	-12	C	0.388	3426.7922	-38	H	0.164
3466.6632			0.008	3447.1842			0.016	3426.5820	-35	H	0.012
3466.1033	6	C	0.030	3447.1340			0.023	3426.1866	-17	H	0.145
3465.9498	-31	H	0.085	3447.0774	3	C	0.129	3425.0169	-5	H	0.044
3465.1480			0.109	3446.9416	2	C	0.171	3424.7243			0.009
3465.0148			0.020	3446.8847	1	C	0.126	3424.3059	1	H	0.014
3464.7416			0.010	3445.8354			0.008	3424.0872	5	C	0.034
3464.6684	3	C	0.297	3445.2200	3	C	0.061	3424.0323	-15	H	0.010
3464.6190			0.014	3445.1581	4	C	0.193	3423.5548	3	H	0.058
3464.3807	4	C	0.100	3443.5415			0.028	3423.2784	7	C	0.149

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3423.2446	-4	C	0.054	3398.9029	-40	H	0.059	3374.0200			0.018
3423.1158	-9	C	0.287	3398.8129	-3	C	0.015	3373.9318			0.111
3422.6135	-19	H	0.024	3398.1450	10	H	0.072	3373.8742	2	H	0.159
3422.3687	-2	C	0.024	3397.2137	6	C	0.240	3373.3589			0.005
3422.3322	-5	C	0.108	3396.8542	-37	H	0.016	3372.8267	-6	H	0.062
3421.7394	6	C	0.101	3396.1727	-11	C	0.015	3371.6998	-2	H	0.026
3420.9527	-4	H	0.055	3395.8575			0.010	3371.1870	-12	H	0.019
3420.5387			0.058	3395.3191			0.011	3371.0213	-3	H	0.200
3420.4981	0	C	0.317	3393.6894	-7	H	0.326	3370.9019	-1	H	0.158
3419.9503	0	C	0.104	3393.5281	-7	H	0.064	3370.2678	5	H	0.053
3419.4618	-1	C	0.047	3393.4743			0.010	3369.9544	-31	H	0.010
3419.1804	54	H	0.011	3393.2154	75	H	0.084	3369.7524	-43	B	0.006
3419.1335			0.006	3393.0065	-55	H	0.223	3369.1527	-16	C	0.014
3419.0498			0.018	3392.9415	-1	C	0.168	3369.1221	2	H	0.028
3418.7762			0.008	3392.7258	3	C	0.060	3368.8206	15	C	0.060
3418.4557	0	C	0.017	3392.6776	111	H	0.012	3368.5267	-14	H	0.149
3417.8553			0.010	3392.5069	-1	C	0.069	3368.4698			0.009
3417.7497			0.011	3392.4256	5	C	0.014	3368.2966	-5	H	0.170
3417.4263			0.010	3391.7496			0.014	3367.8145	-20	H	0.043
3416.1588	-26	H	0.405	3391.7127	-119	H	0.009	3367.6430	3	C	0.104
3415.6664			0.100	3391.5703	-11	C	0.065	3367.5194	3	C	0.017
3415.5897			0.007	3391.5132			0.014	3366.5357	-6	C	0.011
3415.5365	-43	H	0.370	3391.4243	3	H	0.213	3366.3769	-74	H	0.010
3414.9725	3	H	0.050	3391.3393	-106	H	0.070	3365.7365	-7	C	0.056
3414.4690			0.008	3391.2662	-8	H	0.014	3365.2794	-17	H	0.009
3414.0304			0.102	3391.0742	60	H	0.071	3364.9036	-16	C	0.014
3413.9906	-15	H	0.299	3391.0473			0.071	3364.8272	-5	C	0.036
3413.9018	-18	H	0.311	3390.1337	-3	H	0.145	3364.7447			0.006
3413.8518			0.145	3387.6205	18	H	0.009	3364.7010	-43	H	0.030
3413.5669			0.120	3387.3778	-2	H	0.098	3364.3464	-7	C	0.019
3413.5354	-127	H	0.070	3385.9960			0.011	3364.2463	2	C	0.010
3413.0675	1	C	0.030	3385.7101	3	C	0.042	3363.4902	-17	H	0.008
3412.4733	33	B	0.014	3385.6745	119	H	0.053	3362.9305	-26	C	0.004
3411.8526	-12	H	0.209	3385.6015	-5	C	0.042	3362.2827	-5	C	0.080
3410.8078	-9	H	0.032	3385.4657	3	H	0.025	3361.6725	0	C	0.143
3410.5757	20	H	0.011	3384.4900	-70	H	0.008	3361.2077			0.022
3410.2043	7	H	0.068	3384.3868	-2	C	0.109	3361.1773			0.071
3409.2013			0.009	3384.1135	1	H	0.194	3360.4805			0.007
3408.8552	-5	C	0.009	3383.1507			0.008	3360.1748	1	C	0.016
3408.1424			0.014	3383.0762	6	C	0.030	3359.7996	-26	H	0.117
3408.0379			0.014	3382.9092			0.020	3359.5196	-1	C	0.056
3406.6750	11	C	0.028	3382.4746			0.165	3359.1532			0.006
3406.5297	3	H	0.011	3380.9168	18	H	0.014	3358.4916			0.004
3405.2545			0.008	3380.4678	7	C	0.022	3357.9325	-5	H	0.020
3405.1826			0.009	3380.2608	37	H	0.037	3357.0339	-3	C	0.082
3404.1483	22	C	0.010	3380.1707			0.035	3356.9063	6	H	0.033
3403.7144	8	C	0.008	3379.6656	45	H	0.019	3355.8981			0.008
3403.5831	1	C	0.042	3379.1239	6	C	0.010	3355.8779	23	H	0.020
3403.4280			0.008	3378.9169			0.025	3355.7059	-1	C	0.113
3402.0853	16	C	0.008	3378.4373	-13	C	0.067	3355.6044	15	H	0.079
3401.4988	-10	C	0.084	3378.0639	-2	C	0.086	3355.1870	20	C	0.011
3401.0917	-8	C	0.038	3377.5495	-1	C	0.013	3354.5258	-7	H	0.028
3401.0536	2	C	0.112	3377.0309			0.040	3354.2974	-31	H	0.082
3400.6502	-13	C	0.035	3375.6194	-13	C	0.006	3353.2839			0.007
3400.5651	-23	H	0.138	3375.4217			0.009	3353.2280	0	C	0.006
3400.4063	-8	H	0.046	3375.2866			0.006	3352.9713	35	H	0.009
3399.7528	-2	H	0.327	3375.1862	-17	H	0.076	3352.6397	-44	H	0.031
3399.5470			0.006	3374.6832	5	C	0.011	3351.6217	-11	H	0.156
3399.4919	-25	H	0.045	3374.3319	-21	H	0.036	3350.6474			0.006
3398.9973	13	H	0.037	3374.0981	79	H	0.009	3350.2492	-2	H	0.039

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3349.6744	-31	H	0.021	3325.7189			0.006	3298.4480			0.008
3348.4443	13	C	0.021	3325.6637			0.010	3298.1529	-10	H	0.007
3348.2117			0.087	3325.1386	-15	H	0.093	3298.1072	3	C	0.069
3348.1698	-30	H	0.141	3324.8659	-12	C	0.011	3297.5037	-4	C	0.028
3347.9897			0.007	3324.5395	-17	C	0.032	3297.1360	-15	H	0.020
3347.4279			0.038	3324.3844	73	H	0.081	3296.6451	2	H	0.040
3347.3812	66	H	0.112	3324.3388	18	H	0.028	3296.4863			0.007
3347.3218			0.030	3324.3037			0.015	3294.8842	-28	H	0.026
3347.2400			0.011	3324.0061	-5	C	0.007	3294.2518	-7	H	0.006
3346.7971	-42	H	0.054	3323.3406			0.010	3294.2107	10	C	0.011
3346.0387	17	C	0.007	3323.1581	-30	H	0.019	3294.0588	16	C	0.016
3345.9896	22	H	0.024	3323.0932			0.007	3293.4284			0.009
3345.8623			0.006	3323.0197	15	C	0.010	3293.3365	-25	H	0.013
3345.8277	-7	H	0.032	3322.2828			0.017	3293.0926	-3	C	0.008
3345.7329	-44	H	0.020	3322.2528	28	H	0.020	3292.8213	-9	C	0.018
3345.3944	56	H	0.105	3322.1908	-1	H	0.068	3292.6199			0.012
3345.3369			0.014	3322.1233	-37	H	0.088	3292.5043	-3	C	0.018
3345.3009	-29	H	0.136	3320.8207	5	H	0.044	3291.3574	4	C	0.051
3344.9935	-5	H	0.121	3320.4849	8	H	0.063	3290.3475			0.005
3342.6067			0.008	3320.0140	24	H	0.009	3290.2011	8	H	0.060
3342.2940	-4	C	0.023	3318.5088	-11	C	0.006	3288.9193	8	C	0.015
3341.3835	6	C	0.024	3317.2799	13	C	0.059	3288.6285			0.005
3340.6323			0.011	3316.0869			0.032	3288.5512	-36	H	0.009
3340.2993	9	C	0.016	3315.8711	-111	H	0.019	3288.4828	4	C	0.019
3340.1392	-13	C	0.007	3315.0444			0.009	3288.2039	17	H	0.012
3339.8840			0.010	3314.1045	-6	H	0.032	3288.0982	-58	H	0.022
3339.7615	-5	H	0.010	3313.9270	-22	H	0.013	3287.2464			0.007
3338.9864	6	C	0.007	3313.3936	-5	C	0.016	3286.1696	-4	B	0.007
3337.1386			0.010	3313.2529	-1	C	0.035	3285.8200	-50	H	0.021
3336.8982	8	C	0.047	3312.0539	-10	C	0.017	3285.7587	-25	H	0.010
3336.8462	2	C	0.222	3311.5844	44	H	0.008	3285.6724	-35	H	0.038
3336.7131	-3	C	0.029	3310.8553	-35	H	0.028	3285.0515			0.009
3335.0691	-2	H	0.056	3310.5257	-3	C	0.146	3285.0002	0	H	0.013
3334.9856			0.017	3309.3807	18	H	0.070	3284.5737			0.007
3334.6297	7	C	0.168	3309.2556	-37	H	0.067	3284.2253	10	C	0.082
3334.5613			0.030	3309.0098	3	C	0.037	3284.1947	-53	B	0.027
3334.4457	20	H	0.016	3308.9842	108	H	0.014	3284.1272			0.007
3334.3726			0.007	3308.8879	6	H	0.013	3283.7627	-4	C	0.050
3334.3355	-26	H	0.028	3308.7816	-87	H	0.042	3283.0617	1	C	0.146
3333.0461	-9	H	0.013	3308.6990	2	C	0.047	3282.9735	-18	H	0.028
3332.6044			0.022	3308.6459			0.015	3282.8341	48	H	0.019
3332.5779			0.070	3308.3201	7	C	0.014	3281.8153	13	H	0.014
3332.5194			0.015	3308.0774	-5	C	0.041	3281.0207	33	H	0.008
3331.8128	15	H	0.021	3307.1865	3	H	0.017	3280.9850			0.005
3331.7341			0.006	3305.2004	1	H	0.066	3280.8931	18	H	0.037
3331.5851			0.007	3305.1391	-109	H	0.027	3280.0739	1	C	0.018
3330.9834	-13	H	0.032	3304.1393	1	H	0.009	3279.3709	-10	H	0.018
3329.6441	-3	C	0.041	3303.9898	12	H	0.019	3279.2590	6	H	0.006
3328.7753			0.008	3303.5464	-59	H	0.006	3279.0964	4	C	0.088
3328.4251	22	H	0.033	3303.2844	4	C	0.008	3278.5655	12	H	0.038
3328.2553	-27	H	0.022	3303.0730	-21	C	0.008	3277.8246			0.007
3327.5875	-8	C	0.034	3302.2088	-41	H	0.014	3277.7026	9	H	0.032
3327.3282	-16	C	0.017	3301.9369	2	H	0.060	3277.6126	-21	H	0.022
3327.0456	0	H	0.085	3301.2152	15	H	0.051	3277.2418			0.010
3326.7963	7	C	0.016	3300.2143	-4	C	0.020	3276.5108	-3	C	0.068
3326.4248	4	C	0.021	3300.1371	3	H	0.013	3276.2206	0	C	0.027
3326.0436	11	C	0.032	3299.8669	-23	H	0.011	3275.9304	7	H	0.007
3326.0102	47	H	0.016	3299.5255			0.005	3275.4752	-13	H	0.034
3325.9447			0.007	3298.9427	33	H	0.046	3275.2575	2	H	0.036
3325.8379	33	H	0.089	3298.7726	-22	H	0.057	3275.1744	-13	C	0.030

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3274.6411			0.020	3253.5849			0.005	3230.3346			0.006
3273.8756			0.008	3252.4192	-8	H	0.005	3230.2842			0.030
3273.7737	-3	C	0.061	3251.8880	-5	H	0.027	3229.9006	1	C	0.029
3273.7311			0.007	3251.7863			0.005	3229.8005			0.003
3273.4273	3	C	0.020	3251.5812	-11	H	0.027	3229.0401	15	C	0.071
3273.4035			0.030	3251.5080			0.013	3228.9081	-59	H	0.003
3272.0506			0.015	3250.2944	19	H	0.006	3228.4654			0.003
3271.6903	-4	C	0.007	3249.6760	-21	H	0.003	3228.1683	3	H	0.017
3271.6758	17	H	0.013	3249.4733			0.003	3228.0658	-37	H	0.012
3271.4694	-26	H	0.007	3249.1963	-31	H	0.026	3227.7506	-7	H	0.016
3271.4437			0.006	3248.9255			0.004	3227.4644			0.045
3271.0717			0.007	3247.3635	12	C	0.038	3226.0686	6	C	0.008
3271.0198	1	C	0.009	3247.2960			0.011	3225.7059	-4	C	0.012
3270.4269	3	C	0.012	3246.5555			0.022	3225.5614	27	H	0.004
3270.1072	-64	H	0.005	3245.4024	2	C	0.013	3223.4563			0.003
3269.0445	36	H	0.017	3244.9427	3	C	0.086	3222.0339	-8	C	0.014
3269.0019	-81	H	0.006	3244.6389	6	H	0.007	3221.2935			0.007
3268.4134			0.005	3244.4063	2	C	0.005	3220.7764			0.003
3267.6235			0.003	3244.1743	-45	H	0.005	3220.4425	0	C	0.020
3267.4835	-3	H	0.034	3243.3657	31	H	0.011	3220.2937			0.013
3267.3754			0.008	3243.2575	-149	H?	0.004	3220.0835			0.003
3266.6836	39	H	0.002	3243.1606	-26	H	0.015	3219.3838	0	C	0.062
3266.3853	-3	C	0.005	3243.0449	-8	C	0.020	3219.2881	-33	H	0.006
3266.0864			0.015	3242.9530			0.005	3218.9416			0.004
3265.9120	-12	H	0.041	3242.6966	-8	H	0.011	3218.7596	49	C?	0.011
3265.5699	-4	H	0.014	3241.7741	2	C	0.008	3218.7140			0.003
3265.3141			0.002	3241.7524	-12	H	0.004	3217.5510	-1	H	0.010
3265.0921	2	C	0.022	3241.4235	-31	H	0.025	3217.3934	40	H	0.004
3264.3901	64	H	0.006	3240.4923	33	H	0.013	3217.3606	-75	H	0.004
3263.4903	-15	H	0.018	3240.1765	-35	H	0.004	3216.5226	5	C	0.015
3263.4249			0.004	3240.1071	1	C	0.028	3216.3940			0.003
3263.2738	-10	C	0.015	3239.6049	27	H	0.007	3216.2458	10	H	0.009
3262.5822	-10	H	0.013	3239.2134			0.008	3215.3199			0.008
3262.5171	1	C	0.003	3239.0970			0.002	3215.0870	-26	H	0.002
3262.4252	-3	H	0.007	3238.8766	-18	H	0.004	3214.5616	5	H	0.013
3262.0687	-18	H	0.022	3238.3501			0.009	3214.1222	-9	C	0.071
3261.8298	2	H	0.033	3238.0262	1	H	0.019	3214.0341			0.011
3261.1626	-4	H	0.031	3237.7396	64	H	0.030	3213.7502	6	H	0.014
3261.0144			0.010	3237.3426			0.012	3213.6383			0.002
3260.4265	-9	C	0.028	3237.0557	18	H	0.011	3213.4069	-9	H	0.017
3260.1644			0.003	3236.9725			0.011	3213.1505			0.005
3259.7031			0.004	3236.8705			0.004	3212.2469			0.007
3259.5377	-45	H	0.004	3236.6492	2	C	0.032	3211.6204			0.007
3258.8920	-23	H	0.004	3236.3996	-14	C	0.017	3211.5860			0.003
3258.2723	-3	H	0.030	3236.2108			0.003	3211.5558			0.017
3258.1585			0.022	3235.4523	-31	H	0.002	3211.3884			0.004
3258.0734	1	C	0.055	3235.1333	3	H	0.015	3210.8587	-9	H	0.011
3257.7068	-18	H	0.010	3234.6936	30	H	0.003	3210.6778			0.015
3257.5544	11	H	0.003	3234.6099	-61	H	0.006	3210.2240			0.004
3257.2254	-7	C	0.034	3234.3704	13	H	0.021	3210.1126			0.010
3257.0730	7	H	0.008	3233.9902	-62	H	0.013	3209.7461	-4	C	0.060
3256.2444	-15	H	0.022	3233.4836			0.005	3208.8070	-1	H	0.054
3256.0837	-16	C	0.124	3233.0192	0	C	0.025	3207.5511			0.007
3255.9988			0.006	3232.8889			0.008	3207.4875	-7	H	0.011
3255.0293	-14	H	0.027	3232.7565	-14	H	0.046	3206.7283	-23	H	0.006
3254.6228	-22	H	0.002	3232.2737	-3	C	0.006	3206.6170			0.003
3254.1483	-1	C	0.077	3231.3313	-17	H	0.018	3206.3337			0.005
3254.0375	41	H	0.025	3230.9836	9	C	0.113	3205.7478	-27	H	0.004
3253.9430	7	H	0.009	3230.5152	47	H	0.016	3204.3327	-8	H	0.010
3253.6818	-1	H	0.017	3230.4201	-7	C	0.048	3203.7707	-3	H	0.009

WAVENUMBER IN CM^{-1}, DIFFERENCE IN 10^{-4}CM^{-1}, INTENSITY IN (TORR-M)$^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3203.4647	-1	C	0.088	3175.2521		M	0.005	3148.1063			0.004
3203.3252	-3	H	0.011	3175.0746	1	H	0.037	3146.5548			0.004
3202.5386	26	H	0.007	3174.8263		M	0.003	3145.8945			0.013
3202.1042	12	H	0.052	3174.7837			0.003	3145.4130			0.004
3202.0119			0.018	3174.6940		M?	0.007	3145.1866			0.003
3200.9711			0.004	3174.5359		M	0.003	3142.8637	41	H	0.003
3200.9236			0.011	3173.1573	-3	C	0.003	3142.7798	2	C	0.011
3200.8348			0.006	3172.5973			0.004	3142.1316			0.007
3199.7254	11	C	0.009	3172.1848			0.004	3140.6286		M	0.016
3199.0745			0.002	3170.2332			0.006	3140.2914		M	0.003
3197.6644	-7	C	0.068	3170.0769			0.008	3140.2196		M	0.009
3196.6457	12	C	0.002	3169.8208	18	C	0.005	3140.0894	9	H	0.014
3196.0931	-5	C	0.018	3169.2729			0.003	3140.0685		M	0.011
3195.6076	35	H	0.008	3167.9098	-9	C	0.006	3140.0439		M	0.003
3195.4813			0.007	3167.5376	28	H	0.005	3140.0195			0.006
3194.6605			0.006	3167.2368			0.002	3139.9920		M	0.013
3194.0386	-9	H	0.005	3167.0592			0.004	3139.7276			0.002
3193.3421	-17	H	0.008	3166.7302		M	0.004	3139.5240	-10	H	0.003
3193.2233			0.002	3166.4559			0.022	3139.1139	-37	H	0.022
3192.2269			0.006	3166.2983		M	0.005	3139.0128	-22	H	0.005
3192.1036	121	H	0.033	3166.1138		M	0.008	3138.1404	-68	H	0.007
3192.0145		M	0.005	3165.4609			0.007	3137.6564			0.007
3191.9720			0.016	3164.4901	-18	H	0.006	3135.3808			0.005
3191.5648	53	H	0.006	3164.3684			0.010	3135.0969	14	H	0.043
3191.3935		M	0.004	3164.0313	-67	H	0.021	3134.6291			0.009
3191.1266			0.002	3163.1654	14	H	0.007	3134.4984			0.007
3190.9415	30	H	0.059	3162.1298			0.009	3133.5694			0.010
3190.1710			0.006	3162.0841			0.005	3133.0685	-15	C	0.076
3189.2311	-17	H	0.009	3160.9985	-15	H	0.003	3132.1598	-4	H	0.002
3189.1316	-35	H	0.003	3159.3446	-19	H	0.004	3131.7364		M	0.019
3188.8379	9	H	0.011	3159.0002	-30	H	0.003	3131.4006	6	H	0.008
3187.5341	46	H	0.027	3158.4222			0.004	3131.3825	1	H	0.017
3186.8112			0.005	3158.1262		M	0.006	3131.3493	16	H	0.033
3186.6907	-38	H	0.006	3157.6955		M	0.005	3131.2626		M	0.004
3186.2709	-13	H	0.005	3157.5762			0.007	3131.2430	-1	H	0.012
3185.2550	0	C	0.029	3157.5506		M	0.003	3131.2061	-2	H	0.007
3185.2090			0.009	3157.5143		M	0.006	3131.1724	-2	H	0.014
3185.1408			0.007	3156.6926	-54	H	0.014	3130.3971			0.009
3184.8240	1	C	0.010	3156.3282	8	H	0.004	3129.9230			0.007
3184.5288			0.004	3155.6182			0.005	3129.5991			0.018
3183.4889	-8	H	0.006	3155.3801	6	H	0.004	3128.5591	4	C	0.009
3183.2680		M	0.003	3154.3514			0.002	3128.3102			0.004
3182.9567		M?	0.006	3153.2808			0.004	3128.1001			0.003
3182.9298	40	H	0.006	3153.1332	-4	H	0.059	3127.8515			0.002
3182.8191			0.007	3152.7255			0.003	3127.4174	-19	C	0.002
3182.7028			0.003	3152.4242			0.008	3126.9156	13	C	0.014
3182.2788			0.002	3152.2811			0.003	3126.7852	-1	C	0.030
3181.6746	13	H	0.002	3152.1016			0.004	3126.5701	15	C	0.007
3181.0801	-54	H	0.074	3151.3555	4	C	0.007	3126.0016	-11	C	0.011
3180.4104			0.006	3149.8940			0.004	3125.1830	-55	H	0.045
3180.3791	-75	H	0.010	3149.5401			0.007	3125.1319	1	C	0.025
3179.6453	-4	H	0.007	3149.4213		M	0.005	3125.0186			0.004
3178.9559			0.004	3149.2599	9	H	0.028	3124.1970	-11	H	0.007
3178.1192	-2	C	0.075	3149.0404		M	0.009	3123.4096			0.004
3177.2579			0.020	3148.9954			0.004	3123.3415			0.004
3177.1298			0.005	3148.8567		M	0.003	3123.1309	5	C	0.011
3177.0394	-14	H	0.005	3148.8234		M	0.010	3123.0672	-10	C	0.004
3176.7390			0.002	3148.7867		M	0.009	3122.7955	-1	C	0.024
3175.8997	18	H	0.067	3148.3508	-20	H	0.039	3122.7643	3	H	0.045
3175.4016	44	H	0.015	3148.2976			0.008	3122.4701	-3	C	0.072

WAVENUMBER IN CM^{-1}, DIFFERENCE IN $10^{-4}CM^{-1}$, INTENSITY IN $(TORR\text{-}M)^{-1}$

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3122.4416		M	0.024	3099.5067			0.004	3067.2349	7	M	0.027
3122.3665		M	0.003	3099.4173			0.003	3067.1638		M	0.039
3122.3317	-1	M	0.023	3098.8163			0.005	3067.1325	-95	H	0.015
3122.2946		M	0.013	3098.6446			0.003	3067.0118	0	C	0.067
3122.2573		M	0.014	3097.9997			0.003	3066.4096	61	M	0.004
3121.9083	-31	H	0.013	3097.2943	6	H	0.035	3066.2708	0	C	0.009
3121.5993	1	C	0.014	3096.9266	3	C	0.025	3065.6173	-6	C	0.011
3120.9646	7	M	0.030	3096.0536			0.003	3064.5638	-13	M	0.007
3120.8902			0.009	3095.9448	-3	C	0.077	3064.4897			0.005
3120.1917			0.020	3095.3713	4	M	0.028	3064.4037	-6	C	0.093
3119.7520			0.003	3095.3513	3	M	0.028	3062.2828			0.002
3119.1817	-4	C	0.015	3095.1793	-1	M	0.050	3061.2292	-9	C	0.009
3118.9803			0.006	3095.1305	-2	M	0.030	3059.9288	-2	C	0.017
3118.9437	-4	C	0.058	3095.1043	2	M	0.020	3059.7230			0.003
3118.1104	6	C	0.038	3095.0596		M	0.030	3059.2590			0.014
3116.6218	-21	C	0.011	3094.5477	0	C	0.009	3058.5575			0.005
3116.0121	-17	C	0.005	3093.8194	-33	H	0.008	3057.9065			0.003
3115.6762	-9	C	0.076	3093.7637			0.004	3057.7601	-8	M	0.037
3114.4931	3	C	0.018	3093.6893	-1	C	0.015	3057.7257		M	0.038
3114.1823			0.003	3093.5692	-67	H	0.022	3057.6879		M	0.063
3113.2102	4	M	0.034	3092.8595	78	H	0.008	3057.5982			0.005
3113.5795			0.005	3092.4317			0.006	3057.1466	2	C	0.007
3113.4181	-3	M	0.020	3090.4826			0.005	3056.3561	-8	C	0.091
3113.3800	-2	M	0.031	3088.9680	12	H	0.002	3055.6097	-3	C	0.009
3113.3023		M	0.018	3088.4016			0.006	3054.4803			0.003
3113.2798		M	0.018	3088.3184	-42	H	0.004	3054.1938			0.008
3113.2615		M	0.031	3087.1915	-6	C	0.024	3051.7677			0.004
3113.1238			0.008	3086.1333			0.006	3051.7345	-55	H	0.016
3112.7029			0.015	3086.0878		M	0.017	3050.7032			0.003
3112.6706			0.007	3086.0715	-2	M	0.034	3050.0734			0.003
3112.5879			0.011	3086.0303	-2	M	0.058	3049.0448	5	C	0.017
3112.5422			0.005	3085.8935	2	M	0.036	3048.9468	-6	C	0.018
3112.3890	-9	C	0.017	3085.8604		M	0.035	3048.6728	0	C	0.028
3112.1839	4	C	0.007	3085.8322		M	0.058	3048.5515	19	M	0.027
3112.0976	10	C	0.012	3085.6897			0.018	3048.1694	2	M	0.019
3110.5911	-26	C	0.004	3085.5071			0.021	3048.1531		M	0.032
3110.3100	21	C	0.013	3085.3588			0.013	3048.0299			0.017
3109.9198			0.004	3083.3029			0.003	3047.7248	-117	H	0.011
3109.7582	0	C	0.013	3082.6061	-9	C	0.029	3047.3721	-31	H	0.017
3109.3774	-4	C	0.006	3082.5561	12	C	0.010	3047.2313			0.005
3108.2406	-8	C	0.015	3082.2522			0.003	3045.6957			0.008
3107.3300	-6	C	0.025	3081.3417	-3	C	0.037	3043.2250			0.003
3107.1499	-12	H	0.032	3080.8639	-98	H	0.004	3042.3358			0.003
3106.0693			0.003	3079.9261			0.005	3042.2670			0.003
3105.6698	-2	C	0.004	3079.6828	-1	C	0.030	3041.9499	-6	H	0.013
3104.5849	-1	M	0.043	3079.5290	0	C	0.037	3041.4309			0.007
3104.3360	-5	M	0.024	3079.3451	-3	H	0.027	3041.2282	-75	H	0.005
3104.2841	3	M	0.024	3077.9374	-9	C	0.031	3039.3961	50	H	0.008
3104.2209		M	0.015	3077.4734	2	C	0.006	3038.4981	-6	M	0.025
3104.2040		M	0.024	3077.0069			0.009	3037.9034			0.003
3103.0153	-2	C	0.029	3076.7250	-5	M	0.038	3037.5801			0.004
3102.7251			0.013	3076.6768	-2	M	0.038	3037.0992			0.006
3102.4600	-18	C	0.008	3076.5693	4	M	0.025	3036.2225			0.007
3102.0629			0.003	3076.5493		M	0.038	3036.0693			0.005
3101.8766	-8	C	0.010	3074.8632			0.003	3036.0024			0.014
3101.4269			0.006	3071.0463			0.001	3035.7822	-12	C	0.023
3101.1555	-4	C	0.067	3069.5157	-5	H	0.025	3034.3953	6	C	0.012
3101.0412	58	M	0.014	3068.9345			0.003	3034.2650	7	C	0.044
3099.8000	-7	C	0.019	3067.3001	-7	M	0.067	3034.1764			0.003
3099.5473	-3	C	0.034	3067.2614	2	M	0.039	3033.5386			0.003

WAVENUMBER IN CM-1, DIFFERENCE IN 10-4CM-1, INTENSITY IN (TORR-M)-1

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
3032.4966			0.004	3015.0914		M	0.013	3005.4548	9	C	0.025
3032.1409			0.011	3015.0508	3	M	0.016	3004.9836			0.002
3031.9903	-12	C	0.021	3015.0020	7	M	0.011	3004.7527			0.003
3031.9563	0	C	0.028	3014.9413	3	M	0.007	3004.6868	7	C	0.034
3031.7342	-2	C	0.072	3014.8381	4	M	0.012	3004.4485		M	0.006
3030.7268	3	C	0.060	3014.7350	0	M	0.021	3003.8375	-4	C	0.014
3029.9098			0.004	3014.7112	-5	M	0.033	3003.4748	3	C	0.009
3028.9050			0.003	3014.6418	3	M	0.022	3002.8529		M	0.002
3028.7519		M	0.026	3014.4886	16	H	0.007	3001.1913			0.004
3028.2365			0.005	3014.3441		M	0.010	2999.6080			0.009
3027.7825			0.010	3014.2760		M	0.006	2999.1578			0.012
3027.3157			0.002	3014.1703	-17	M	0.012	2999.0605		M	0.009
3027.1271			0.003	3014.0951	-5	M	0.011	2998.9943		M	0.013
3027.0146	-36	H	0.002	3014.0608	6	M	0.009	2998.9717			0.003
3026.9610			0.003	3013.8068	5	M	0.008	2997.2872	-42	H	0.007
3025.7603	-8	C	0.029	3013.7235	0	M	0.014	2996.3926			0.003
3025.4189			0.003	3013.7099	-2	M	0.012	2995.4556	7	C	0.016
3024.3695	-3	H	0.011	3013.5921		M	0.011	2994.7208	-1	H	0.015
3024.1526			0.003	3013.5716	-17	C	0.019	2994.4469	2	C	0.045
3023.8101			0.012	3013.5132		M	0.009	2993.7352	-17	C	0.021
3023.1494			0.016	3013.4078		M	0.007	2992.6542	10	C	0.018
3022.6651			0.008	3013.1649		M	0.011	2991.9707	5	C	0.011
3022.3646	-17	C	0.012	3013.1269	-2	M	0.009	2991.2553	25	H	0.005
3021.7693	-15	H	0.020	3013.0780	-1	M	0.014	2990.6724			0.003
3019.2121	6	H	0.023	3012.9170	8	M	0.006	2989.7151			0.005
3019.0961			0.003	3012.8527	6	M	0.005	2989.6238			0.006
3018.8241			0.015	3012.7105		M	0.005	2989.5969	-23	H	0.017
3018.6496	-5	M	0.023	3012.6174	-12	M	0.031	2989.0335	0	M	0.020
3018.5908		M	0.015	3012.5308	-4	C	0.054	2988.9322	-2	M	0.020
3018.5283		M	0.046	3012.5036		M	0.005	2988.7946		M	0.032
3018.3576	-12	M	0.027	3012.3762	-4	C	0.015	2988.6114	-16	C	0.011
3018.2418	-2	M	0.028	3012.3431			0.004	2988.2875			0.011
3018.2055	1	M	0.032	3012.2305			0.022	2988.2393			0.010
3017.8853	-2	M	0.019	3012.0645			0.015	2988.1905			0.004
3017.8267	15	M	0.020	3012.0285	-6	M	0.005	2987.7384	-11	H	0.005
3017.8149	-4	M	0.027	3011.9291	-1	M	0.005	2987.5245	0	C	0.033
3017.7631	2	M	0.021	3011.8214	-4	M	0.004	2987.0117			0.004
3017.7106		M	0.050	3011.7986		M	0.003	2984.2115	-2	C	0.004
3017.4669		M	0.047	3011.5966		M	0.002	2983.3149			0.006
3017.3452	-4	M	0.028	3011.4345	0	M	0.017	2982.4526			0.005
3017.2608	4	M	0.030	3011.2775	-2	C	0.008	2981.3631			0.007
3017.2281	2	M	0.027	3011.2400		M	0.003	2981.2394			0.003
3017.1624	-8	M	0.031	3011.0261			0.009	2981.1706			0.004
3017.1036			0.004	3010.9104	-14	M	0.007	2981.1437	-1	C	0.017
3016.9385	-9	M	0.025	3010.8825		M	0.007	2980.6755			0.006
3016.7330	0	M	0.017	3010.6699		M	0.005	2980.3879	7	C	0.022
3016.6404	0	M	0.024	3010.6002		M	0.003	2980.2403			0.008
3016.5641	-15	M	0.046	3010.2321	-2	C	0.044	2979.7481			0.008
3016.4954	-10	M	0.047	3010.1772	-8	M	0.022	2979.0701			0.007
3016.4585	4	M	0.018	3009.6543	24	C	0.007	2979.0113		M	0.038
3016.3684	-4	M	0.020	3009.5336		M	0.003	2978.9194	-7	M	0.023
3016.3015	0	M	0.013	3009.0114		M	0.005	2978.8475	-5	M	0.017
3015.9894	1	M	0.020	3008.8501		M	0.009	2978.6507	1	M	0.023
3015.8062	7	M	0.029	3008.4002		M	0.007	2977.9426	-9	C	0.021
3015.7062	0	M	0.016	3008.2779			0.007	2977.4768	-18	H	0.013
3015.6824	0	M	0.023	3007.6932			0.003	2975.3795			0.007
3015.6411	-6	M	0.024	3007.4505		M	0.011	2975.2938			0.009
3015.6155	1	C	0.059	3007.0780		M	0.003	2975.2225			0.005
3015.5911	4	M	0.015	3005.9804		M	0.006	2975.0837	-2	C	0.034
3015.2034	5	M	0.027	3005.7271		M	0.005	2974.8305			0.005

WAVENUMBER IN CM-1, DIFFERENCE IN 10-4CM-1, INTENSITY IN (TORR-M)-1

WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT	WAVENUMBER	DIFF	CD	INT
2974.5886	-14	C	0.013								
2973.7212			0.007								
2973.2534	11	C	0.024								
2972.0533			0.004								
2971.7158			0.003								
2970.5320	-16	H	0.003								
2969.5158			0.014								
2968.8557	5	H	0.024								
2968.7353		H	0.024								
2968.4736	3	H	0.016								
2968.4034	-1	H	0.023								
2967.9841			0.005								
2967.4400	-8	H	0.011								
2966.8341			0.004								
2966.7337			0.003								
2966.0064	-6	C	0.023								

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high temperature water vapor spectrum

tunable difference-frequency laser spectrometer

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The absorption spectrum of water vapor has been recorded at very high temperatures (~1200 K) in the 3000 to 4000 cm^{-1} region with Doppler-limited resolution using a tunable difference-frequency laser spectrometer. This region encompasses the strong OH stretching fundamentals and the bending overtone. The higher rotational and vibrational energy levels observed here are expected to lead to extended theoretical models of H_2O which are necessary to predict and analyze spectra from high temperature combustion processes.

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